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Modelling CO₂ Transport and the Effect of Impurities: A New Equation of State for CCS Pipeline Transport

A thesis submitted to the University of Nottingham
for the degree of Doctor of Engineering

Thomas Alexander Demetriades

Supervisors: Prof. Trevor Drage, Dr. Richard Graham

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“If you want to get from A to B
I’ll give you this advice for free:
You’ll find that cycling in the snow
Is not the quickest way to go!”

— Colin McNaughton

Acknowledgement

I am fortunate to have enjoyed a multitude of fantastic experiences whilst working on this EngD, having spoken with many interesting people, having had the opportunity to travel far-and-wide, and having found a niche for my skills. There have been good times that I shall remember with fondness, and tough times that I will try to use to make myself better. My journey has been an enjoyable one, and I cannot believe this part of my life is over already.

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Abstract

In this EngD project I developed a new, analytic equation of state for use in the area of CCS pipeline transport. It was my aim to design a model which would exhibit a high degree of accuracy within the anticipated window of operation of CCS pipelines; from 260 to 335K and 1 to 200bar, whilst simultaneously retaining a simplicity and ease-of-use, a lack of which made some other available equations particularly unwieldy. Having conducted a comprehensive literature review and attended many academic and industrial conferences throughout this project, I felt that there was a need for an equation of state which could perform both these functions. This was the key motivation for my work, and the model presented in this thesis was developed in order that it might contribute towards negating the many concerns that currently surround the pipeline transport stage of CCS.

I aimed for the proposed model to display a complexity approaching that of some of the simpler equations currently available, whilst incorporating sufficient flexibility to give thermodynamic predictions to a standard approaching that of those which are more complicated. I defined criteria by which the proposed model could be judged, so that it could be applied with confidence in the determination of the physical properties of carbon dioxide mixtures during CCS pipeline transport.

Work was carried out by fitting the parameters of the proposed model to experimental data gathered from the literature, so that it would be able to determine the homogeneous phase pressure and vapour-liquid equilibrium behaviour of carbon dioxide and other relevant gas mixtures. The project yielded a number of excellent outputs, not least the satisfaction of the primary aim which was the proposal of a model, which through this EngD, I demonstrated had the ability to meet the demands that were set. In carrying out this work, I also developed several highly useful auxiliary mathematical methods which helped in ensuring the proposed model was as accurate as possible.

For the case of modelling pure carbon dioxide, the proposed equation worked exceptionally well, providing highly accurate predictions for homogeneous density and vapour liquid equilibrium, which were well within the targets set. A paper on this was published in May 2013. In extending the model to incorporate some binary mixtures I again found that it demonstrated a clear ability to capture the necessary physical behaviours within the target range. I concluded with suggestions as to ways in which the work presented here could be developed further, as well as the many avenues for future work in other areas that this EngD project had opened up.

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List of Mathematical Nomenclature

| | |
|--------------------|--|
| a | Model parameter for the proposed equation of state |
| b | Model parameter for the proposed equation of state |
| c | Model parameter for the proposed equation of state |
| d | Model parameter for the proposed equation of state |
| e | Model parameter for the proposed equation of state |
| f | Model parameter for the proposed equation of state |
| f | Fugacity |
| g | Model parameter for the proposed equation of state |
| G | Gibbs free energy |
| m | Total mass of a system |
| M_r | Molecular mass |
| N | Total number of moles in a system |
| N_i | Total number of moles of substance i |
| N_{rest} | Total number of moles of all substances other than i |
| P | Pressure |
| P_c | Critical pressure of carbon dioxide unless otherwise specified |
| P_{vap} | Vapour pressure; that at which the bubble and dew points occur |
| R | The universal gas constant |
| S | Entropy |
| T | Temperature |
| T_c | Critical temperature of carbon dioxide unless otherwise specified |
| u_i | Bubble point molar volume for substance i |
| U | Internal energy |
| v | Molar volume |
| v_{BP} | The volume at which the bubble point occurs |
| v_c | Critical molar volume of carbon dioxide unless otherwise specified |
| v_{DP} | The volume at which the dew point occurs |
| v_t | Typical molar volume of carbon dioxide unless otherwise specified |
| V | Total volume of a thermodynamic system |
| w_i | Dew point molar volume for substance i |
| W | Weighting constant |
| x | Concentration in the liquid phase |
| y | Concentration in the vapour phase |
| Z | Compressibility factor |
| Z_c | Critical compressibility factor of carbon dioxide unless otherwise specified |
| Γ | Coexistence constraint |
| μ | Chemical potential |
| ξ_{BP} | Bubble constant |
| ξ_{DP} | Dew constant |
| ρ | Density |
| Υ | Dew ratio |
| ϕ | Fugacity coefficient |
| χ_{DP} | Critical constant |
| ω | Acentric factor |
| $*$ | Used to denote a dimensionless quantity |
| \sim | Used to denote an estimated quantity |

Acronyms and Abbreviations

| | |
|------------------|--|
| Ar | Argon |
| BP | Bubble Point |
| CAT | Carbon Abatement Technology |
| CCS | Carbon Capture and Storage |
| CH ₄ | Methane |
| CO | Carbon Monoxide |
| CO ₂ | Carbon Dioxide |
| DP | Dew Point |
| EOR | Enhanced Oil Recovery |
| EoS | Equation of State |
| GHG | Greenhouse Gas |
| H ₂ | Hydrogen |
| H ₂ S | Hydrogen Sulfide |
| Hg | Mercury |
| IEA | International Energy Agency |
| IGCC | Integrated Gasification Combined Cycle |
| IGL | Ideal Gas Law |
| LCO ₂ | Liquefied Carbon Dioxide |
| LIN | Liquefied Nitrogen |
| LNG | Liquefied Natural Gas |
| N ₂ | Nitrogen |
| NIST | National Institute of Standards and Technology |
| NO _x | Nitrogen Oxide |
| O ₂ | Oxygen |
| ppb | parts per billion |
| ppm | parts per million |
| PR | Peng–Robinson (Equation of State) |
| RK | Redlich–Kwong (Equation of State) |
| SATP | Standard Ambient Temperature and Pressure |
| SO _x | Sulphur Oxide |
| SRK | Soave–Redlich–Kwong (Equation of State) |
| SW | Span–Wagner (Equation of State) |
| VdW | Van der Waals (Equation of State) |
| VLE | Vapour–Liquid Equilibrium |

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Chapter 1

Establishing the Need for a New Equation of State

1.1 Environmental Concerns

“Business as usual’ emissions will take greenhouse gas concentrations and global temperatures way beyond the range of human experience. In the absence of action, the stock of greenhouse gases in the atmosphere could more than treble by the end of the century” [1].

The acceleration in industrialisation of the world’s major economies since the middle of the twentieth century has been facilitated by energy from coal-fired power stations and other heavy industry. Until very recently, energy extraction from fossil fuels was neither a clean, nor particularly efficient process, and the damage being done to the environment, encompassing all manner of habitable locations and natural resources needed for the sustenance of life and biodiversity, through the emission of greenhouse gases from large-scale power generation and other heavy industry has begun to be more fully understood [2]. In particular, a strong link between global warming and the release of carbon dioxide (CO_2) during power generation has been identified [3]:

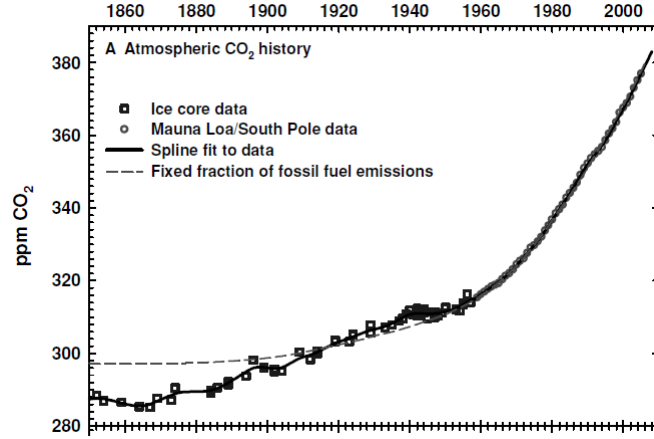


Figure 1.1: Rising levels of atmospheric carbon dioxide

In recent times the first readings of 400ppm atmospheric carbon dioxide have been recorded [4] (see Figure 1.1), signifying that we are now at a watershed moment in terms of the well-being of our atmosphere, and consequently, that a change is urgently needed. Targets of keeping global temperature rises to less than 2°C above 1990 levels by 2050 [5] necessitate that abatement of emissions of all greenhouse gases, of which carbon dioxide is the most abundantly emitted, should become a priority [6].

1.1.1 A Problem Needing A Solution

It is widely agreed that the situation with regard to greenhouse gas emissions from power generation is not sustainable [7]. Targets for an 80% reduction of carbon dioxide emissions by 2050 [6] have resulted in an impetus for investigation into new power generation techniques [5, 6]. It has also partly been due to an awareness that there is an ever-increasing gap between the demand for energy and the capacity of existing power generation facilities. Questions have been raised about the sustainability of previous fossil-fuel power generation methods [8], in terms of their economic viability [1, 9], in terms of preserving resources [10], and in terms of environmental sustainability [8].

In particular, it has become clear that the problem of combating the climate change brought about by industrial-scale power generation and heavy industry such as steel manufacture and cement works is no longer simply a technological one [11]. It incorporates very important considerations including regulatory implementation, economic and financial management, and sociological responsibility. The difficulty of finding a simultaneous solution to the apparently contradictory targets of en-

surging energy security [8], keeping costs low [1], and maintaining carbon emissions reductions [12, 4] forms the basis of this 21st-century energy concern.

The problem stems from the fact that we find ourselves committed to gaining a large proportion of our energy from fossil fuels [11]. Using the combustion of coal, oil and natural gas is such a well-established method of energy extraction that it poses an immense challenge in order to radically alter our habits and obtain energy from a different source. One problem is that although more environmentally friendly and sustainable methods of energy extraction such as wind, tidal and solar power have potentially huge capacity, they are currently nowhere near as dependable as fossil-fuels [13]. Additionally, hopes pinned on the long-term viability of nuclear power have yet to be proven [14], especially in the wake of the Fukushima disaster in March 2011 [15]. As such, relying entirely on any of these alternative technologies could leave massive energy shortfalls. As things stand therefore, these methods are, despite extensive research and development programmes, unsuitable for anything other than contributing small amounts to the overall generation of power.

Of course, it is inevitable that one day, any dependence on fossil fuels will have to cease, as the stock of resources starts to dwindle [11]. On the other hand, it is a reality that for the foreseeable future, while the alternative technologies which one day will provide the entirety of our energy are developed; a process expected to take decades, that the majority of our energy will have to continue to come from fossil fuel sources [10]. It is imperative therefore that during this time, far better use of what is available will have to be made, in terms of efficiency of generation, in terms of reduction of use, and by the minimisation of the environmental impacts associated with its continued and widespread use. These aims appear contradictory, as it would seem to be self-evident that the ability to reduce the environmental impact of power-generation should come at the cost of either reduced efficiency of the overall energy production process, or increased cost to the end user [16].

The reconciliation of the many differences in the necessary requirements of on-going and new generation methods will have to be implemented in such a way as to ensure a long-term viability. Specifically, any medium-to-long term solution which could allow for continued energy extraction from our most abundant energy sources, without the dogmatic long-term disintegration of the Earth's ability to support life, would be of tremendous value.

1.1.2 Carbon Capture and Storage

Carbon Capture and Storage (CCS) is one of the key strategies whose aim is reducing the emissions of Green House Gases (GHG). It is seen in particular as a key carbon abatement technology (CAT), by which it is hoped that the rising levels of carbon dioxide emissions with which we associate environmental destruction can be mitigated [17]. Its place as one of the main strategies for carbon abatement is highlighted by the International Energy Agency (IEA) Blue map, and its importance is highlighted by being mentioned alongside technologies such as nuclear power and biomass, or strategies such as efficiency improvements [17]. Broadly speaking, CCS aims to do this by taking the emitted carbon dioxide and storing it underground. In its most simple form, CCS may be considered a five stage process (see Figure 1.2) whereby these damaging emissions are captured and isolated from the environment [2].

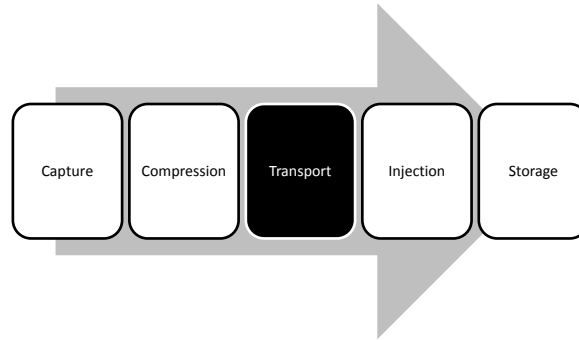


Figure 1.2: The CCS Chain with the transport stage, which is the technical focus of this research project, highlighted

With much development of the underlying technical understanding and of the contextual issues to do with this new technology still required however, CCS is still envisaged to be some way off from being deployed on the scale required to affect a meaningful reduction in carbon emissions.

Capture

The capture phase is where the carbon dioxide is removed from the exhaust stream of the power plant or other industrial process. There are three main ways in which this can be done [8]:

- Post-combustion carbon capture sequesters the carbon dioxide after combustion of the fossil fuel, separating it from the exhaust stream using a chemical

solvent or a physical absorbent.

- Pre-combustion carbon capture, or Integrated Gasification Combined Cycle (IGCC), prevents a release of carbon dioxide into the atmosphere by separating the carbon from the hydrogen in the fuel through a gasification process. From here the hydrogen is used for further power generation after being separated from the carbon dioxide.
- Oxy-fuel combustion involves burning the fuel in an oxygen-rich mixture containing carbon dioxide instead of in air, before some carbon dioxide is removed and some retained to help burn more fuel.

The current state of technological development would suggest that post-combustion capture is the favoured option as it can retrofit onto pre-existing plant and be turned off without affecting generation. It is anticipated however that IGCC will become the favoured option eventually due to cost effectiveness [2]. Either way, the understanding needed to carry out CCS capture is in place, and has been repeatedly demonstrated on different scales (from small to large).

Compression

A conservative estimate of the amount of carbon dioxide released globally from power generation sources in 2000 is 9Gt [5]. Assuming Standard Ambient Temperature and Pressure (SATP); 25°C and 1bar, this equates roughly to $4.581 \times 10^{12} \text{m}^3$. Given that CCS aims eventually to capture 100% of carbon emissions from power plants [18], there is simply no way this volume could be handled unless it could be compressed to a much smaller volume. More importantly, if geological storage is to be used then compression is essential to overcome the reservoir pressures found at depths intended for CCS of around 2km, which in some cases could be as high as 200bar [18]. At its critical point, carbon dioxide is approximately 65 times less voluminous than at SATP, suggesting that CCS must by necessity contain a stage for compression of the captive gases so as to allow a higher quantity to be processed and ultimately isolated from the environment. It is anticipated that compression would usually occur at the same facility as the capture stage. Much research on different compression technologies has been carried out, and it is also likely [19] that CCS-scale compression could be implemented whenever CCS is needed. Yet, it is important to remember that compression is an energy intensive process, requiring in the case of post-combustion capture, as much as 4% of the total energy output

of the power plant [19]. As far the interaction between the compression and transport stages is concerned, compression facilities must be able to meet the pressure requirements of the subsequent stages. It is also important for the operation of CCS systems, particularly when it comes to contingency planning and dispersion modelling in the case of pipeline failure, to be able to understand the compression and depressurisation requirements and behaviour which occurs in CCS. This requirement is explored in more depth later in this thesis.

Transport

Since sources of carbon dioxide are, generally speaking, not in the proximity of the location of the storage sites, some sort of mass transport infrastructure is required to deliver the captured, compressed carbon dioxide gas mixtures to the storage site. Two options for transport are usually considered; pipeline [20, 21, 22, 23] which can be further sub-categorised into on-shore and off-shore pipes, and ship or tanker [21, 24, 25, 26], with each method being employed as determined by locally occurring conditions. Given the geographically disperse nature of sites used for power generation and those which are suitable for the latter stages of CCS, transport infrastructure, particularly pipelines, will be immense structures, for which cost-minimal installation and guaranteed safe operation will be profoundly important. As a direct result of these requirements as well as the fact that transport infrastructure is almost inevitably going to have to be routed close to inhabited areas, the issue of CCS transport is one which is subject to particular scrutiny. With pipelines being the favoured option for transport due to a lower average operating cost for anything other than very long distances (see Figure 1.3), the potentially convoluted planning and construction process, and a perceived lack of ability to guarantee safe operation (for example, as seen in the Barendrecht case, see Figure 1.16 [27]) could inhibit the installation of pipeline infrastructure during the early days of CCS, until this technology has been proven.

As can be seen from Figures 1.3 and 1.4, with the anticipated costs of pipeline transport comparing favourably to those of shipping costs over shorter distances, it is expected to be the favoured option in satisfying the majority of demand for CCS transport.

Injection

The most economically favourable and high capacity sites which have been earmarked for CCS storage are located under ground in geological structures such as

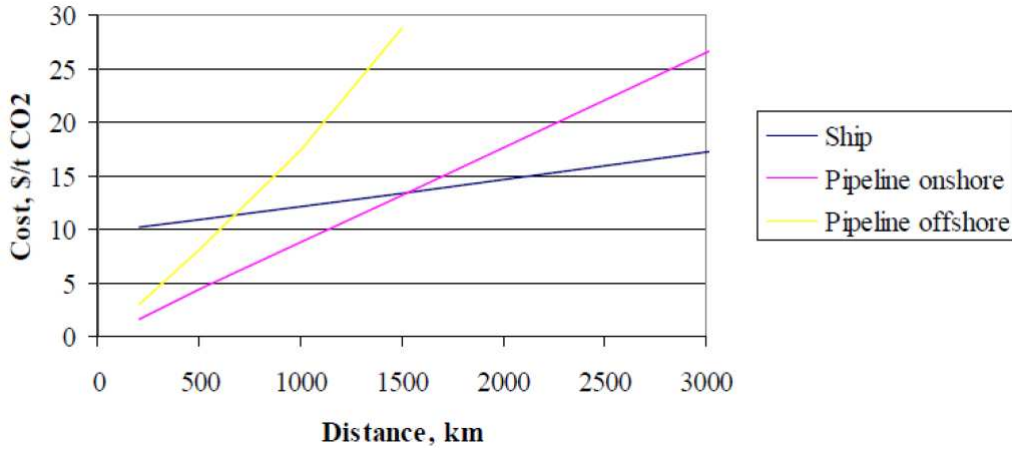


Figure 1.3: Comparison of the anticipated operation costs for different transport methods for a specific volume (6MT) of carbon dioxide [28]

reservoirs or disused oil fields. In order to get the captured carbon dioxide from the transport vessel into the final storage location, it must be injected into the storage site back down the tubing at a high enough pressure to allow the carbon dioxide to overcome the significant pressures found within these formations, and be driven down into the structure. Storage sites must undergo rigorous testing before being allowed to have CO₂ injected. Criteria for storage sites include having a structure that will ensure both minimal migration of the carbon dioxide, and minimal release during seismic activity [8].

Storage and Monitoring

This is the only stage of CCS which requires no active input. After injection, the carbon dioxide remains in place indefinitely and must be monitored to ensure migration to neighbouring geologic formations or potential releases do not occur. In this way, the carbon dioxide is sequestered from the atmosphere and the associated environmental impacts mitigated.

This is a vast simplification of the overall CCS process and the piecemeal presentation given here does not do justice to the overall complexity of the system. In reality the five stages are highly inter-dependent and the interactions between consecutive stages are significant enough that they need to be carefully accounted for [29, 30] in the design of the overall process.

A significant added complexity to the operation of CCS arises from the fact that impure carbon dioxide will have to be processed. In particular, given the range of chemical components found in fossil fuels, for example the different hydrocarbons involved, and specifically the non-hydrocarbon impurities originating from the formation of fossil fuels over many millions of years, as well as different combustion and capture technologies which vary from generator to generator, it is to be expected that CCS capture modules will not produce a pure stream of carbon dioxide. Instead, they will include various chemical impurities which would then be present for the rest of the CCS chain. The thermodynamic effect of these impurities on the overall physical properties of carbon dioxide is profound [31], and there must be scope to understand the effect these have within all the CCS processes. In particular, significant amounts of nitrogen, hydrogen, oxygen, and water could all be found in an untreated fossil exhaust stream. These impurities all affect the physical properties of the carbon dioxide in such a way as to significantly alter the operating parameters of a CCS pipeline, such as wall thickness, diameter, phase behaviour, and pressurisation. A rigorous understanding of the effect of these impurities is essential therefore.

1.2 The Need for An Accurate and Simple-to-Use Equation of State in CCS Pipeline Transport

Many of the most pressing requirements for a timely deployment of CCS seem to be heavily related to the transport stage [32]. Of these, one of the main barriers to overcoming the many political, social and regulatory issues surrounding CCS transport is our lack of ability to accurately predict how the physical properties of carbon dioxide change as the type and amount of chemical impurity varies [31].

Typically, properties such as pressure, density and phase behaviour are calculated using an Equation of State (EoS). This is a formulation relating the important thermodynamic quantities which determine the nature and key characteristics of the system. Presently, there are several available equations of state which could be utilised [33, 34, 35], but all have their relative drawbacks: namely, those which are more accurate are agreed to be also more cumbersome in their implementation, whilst those which exhibit the property of being easier to use fall significantly short of the level of accuracy needed to be of use in CCS.

In particular, there is a clear need at this moment [36], so far as the pipeline transport stage of CCS is concerned, for an equation of state which can accurately depict the key physical behaviours of carbon dioxide-rich gas mixtures in a simple and effective way, without excessive functional complexity or a requirement on high computing power. If such an equation was developed, it would allow safe design and operation of pipelines because it would describe in a quantitative way the variation of pressure, density and phase behaviour as a function of impurity content. This in turn would allow the thermodynamic properties of the system to be evaluated both with increased ease and reduced uncertainty.

As an example, one major area in which there is a direct application of an equation of state in CCS pipeline is in understanding methods of fracture propagation [37, 38]. If CCS pipelines are to be routed through or close to populated areas, the possibility of external influence (for example, diggers or other such heavy machinery) on the pipe resulting in damage cannot be discounted, and so a detailed knowledge of the thermodynamic behaviour before, during, and after failure of pipe is essential. The field of fracture mechanics is particularly dependent on accurate equations of state being available, and deals with how the pipe structure can cope with such external influences [37]. Clearly there is an important safety implication here, and one very clear reason why accurate equations are necessary.

The need for accuracy also pervades cost considerations. Being able to accurately predict the pressures a pipeline will need to undergo given an anticipated impurity stream could save excessive pipe wall thickness being implemented, and in doing so save considerably on the significant capital requirement for CCS pipelines.

As we have identified, there is much that needs to be understood before safe, socially acceptable and cost effective CCS transport networks can be constructed, especially in the prediction of key physical behaviours such as density, pressure and phase behaviour. In light of the pressing need for quick deployment of all the CCS stages, it would seem to be pertinent to ensure that arguments relating to the safe operation of CCS pipelines be neutralised now with the development of a new equation of state which could perform in the ways described here so as to facilitate the high standards of operation required.

1.3 A Contextual Literature Review

1.3.1 Overview of the Literature Surrounding CCS Pipeline Transport

The main aim of this contextual literature review is to establish scope for this EngD research project and to help define our aims. We thus seek to determine the ways that existing equations of state are understood to be lacking, and also to look for the anticipated optimum operating conditions for the pipeline transportation of carbon dioxide so that we can focus our work and ensure its relevance. As established in Section 1.1.2, the principal methods which are likely to possess the required scale for CCS transport are pipelines and ship [26] (see both illustrations in Figure 1.4), with almost no consideration or mention of any other method throughout the entire literature, except for one brief mention of road or rail transport [32], where it also mentions how unsuitable these methods are for large scale transportation. Thus, for the purpose of this project and the current literature review, it will be assumed that there are just these two choices, and that of these, pipeline transport will be the favoured option in the majority of (but not all) cases.



Figure 1.4: The two methods of transport in the CCS process: pipelines (left, [39]), and shipping (right, [26]). Note that most CCS pipelines will be buried below ground. Given the relative lack of CCS pipelines currently, the picture on the left is actually an illustration of an oil pipeline.

Crucially, within the literature, there is a broad consensus that there is currently a lack of any suitable equation of state for specific application to CCS pipeline transport [40, 41]. Also mentioned in the literature is the lack of reliable thermodynamic data for the determination of optimum CCS pipeline transport conditions [29, 30]. The literature also notes that there has been far more study of the other processes

in CCS, notably capture and storage. We are reminded [42] that transport has, in the past, been assumed a problem of inferior difficulty and technical importance, yet we are now facing the very real possibility that the deployment of CCS could be limited to how quickly we can understand the thermodynamics underlying the transport of carbon dioxide [40] and overcome the political hurdles directly arising from this lack of certainty. In the literature, some simulations of the transport process are reported [29], in which particular attention to the upstream interface between capture and transport, including compression, is given, as opposed to the downstream interface of transportation with injection and storage, finding that if energy usage for transport is to be minimised, then the important factors are inlet pressure, amount of impurities in the carbon dioxide, temperature and compressor efficiency.

One of the main issues surrounding CO₂ transport is the need for onshore pipelines. Whichever option is chosen for offshore transportation, routing of pipelines onshore is almost certainly going to cause problems, especially in regions where population density is high, such as in the Humber region of the UK where large-scale CCS projects are expected to be based [43]. One major reason for this is the likelihood with which external influence such as tractors or diggers could cause a pipeline failure; an eventuality whose probability far outweighs that of a failure arising from an internal failure in the pipeline such as corrosion or pressure surge. There are significant problems [44] with how to route the pipeline in such situations, such as social resistances in the form of people not wanting high pressure carbon dioxide pipelines running close to their place of residence, for obvious reasons when considering the possible health effects of exposure to CO₂ (see Section 1.3.2). Such discussions and the reservations of those who live close to the planned route of CCS pipelines are exacerbated in light of the fact that corrosion is a reasonably likely consequence of transportation of supercritical carbon dioxide with water impurity in it [45, 46]. The extent to which it is important to avoid excessive corrosion of the transport vessel ensures that water levels must be kept to a minimum [31], this is to be enforced with strict drying regimes before the carbon dioxide is allowed to enter the pipeline network. The tolerance of water level in the fluid depends on the other chemical components present in the mixture, so it is understood that the quantity of water allowed is likely to be negligibly small. This highlights the requirement for a rigorous and safe pipeline operating procedure with minimal pipeline failure probability. Again, this points back to the requirement for an accurate and easy to use equation of state for use in this area.

Clearly, safety and value for money are considerable issues when it comes to any

of the CCS processes. Given that pipelines will, by their very nature, have to pass through populated areas, a leak from a high pressure carbon dioxide pipeline is likely to cause many problems. The literature notes that since carbon dioxide is heavier than air, if there is a leak it is likely that it will gather in pockets near the ground [47], rather than rise away as might be the case with a natural gas leak. This is particularly problematic for onshore pipelines, with carbon dioxide being an asphyxiant, exposure to anything other than minimal concentrations of which for anything other than very short periods of time can have extremely detrimental health effects [31].

Because of this, it is most important to the safe operation of transportation mechanisms that the pressure, density and phase behaviour of the fluid mixture can be understood. In this way, these characteristics could be accounted for and controlled in order to ensure the pipeline infrastructure does not fail and cause a leak. This eventuality could be brought about in two different ways: Firstly, if the pressure was allowed to become too high this could cause a rupture in the pipeline wall, with the carbon dioxide then being allowed to escape. This suggests that it is important to be able to predict how pressure will vary depending on impurity content and other factors. Secondly, if multi-phase flow is allowed to occur, the difference in viscosity and density of the two phases could weaken the pipeline integrity at valves, pumps, and compressors, situations which again could lead to failure of the pipeline structure. For this reason, it is vitally important that the location of any two-phase region in which both liquid and vapour would coexist should be avoided. It is particularly important to be able to accurately identify where such a two-phase region might occur, given the particular composition of the fluid mixture contained within the pipe. This is because two different phases means two different densities, and therefore two different flow speeds and two different flow regimes, causing damage to the pipeline. Figure 1.5 shows how and where the introduction of a small amount of impurity can create a two-phase region [48].

The literature also lists other key considerations for pipeline operation. For example, it is necessary to avoid formation of solid hydrates or other waxy substances which could disturb the flow rate or cause blockages within the pipe interior [49]. An EoS is again needed for these predictions.

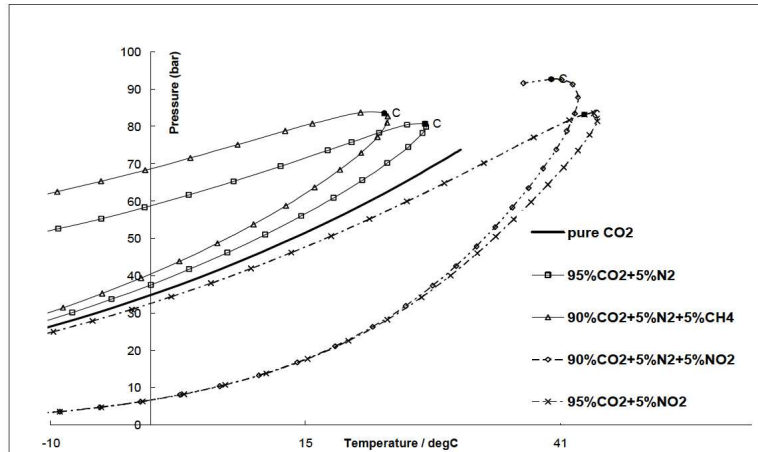


Figure 1.5: Location of the two phase region depending on impurity [48]

1.3.2 Health Impacts of High Concentration Carbon Dioxide

Carbon dioxide is classed as a GHG and its contributions towards global warming are well documented [1, 3]. CCS is a key CAT and it is hoped that in years to come it will help to stop the current pattern of global increases in atmospheric temperature that have been seen in recent decades. There are some other industrial uses for CO_2 which could be utilised in order to help prevent its release into the atmosphere, such as in EOR (enhanced oil recovery) or the food industry [26, 50]. Generally, the amount of CO_2 demanded for these are nowhere near the amount of CO_2 emitted by power plants and other heavy industry, although the lessons learned from EOR in the USA are invaluable for pipeline transportation of CO_2 in CCS as there are several areas of technical knowledge which overlap.

Pure carbon dioxide is a gas at SATP. Despite the fact that it is a key component of our atmosphere, without which life could not exist, in high concentrations it is toxic. The characteristic of carbon dioxide which makes it particularly dangerous to humans, aside from the threat to our atmosphere, is that it is an asphyxiant, restricting the ability of the haemoglobin in blood to transport oxygen round the body. Table 1.1 summarises the health effects of increasing concentrations of carbon dioxide:

From this table we can see why it is vital to prevent a release of CO_2 from pipelines where the quality would be above 90%. This reasoning also determines indirectly

| Concentration | Effects [51] |
|---------------|--|
| < 1% | quite harmless |
| 1–5 % | moderate symptoms such as drowsiness and headache will take effect |
| 5–10 % | effects will become more severe, with dimmed vision, reduced hearing and shortness of breath all possible |
| 10% | symptoms of prolonged exposure become very serious; muscular tremor, increased blood pressure and even unconsciousness |
| > 10% | death within a few minutes |

Table 1.1: Effects on health of increasing carbon dioxide concentration

how far away carbon dioxide pipelines will need to be positioned from inhabited areas. The study of the dispersion of carbon dioxide [37], coupled with the information in Table 1.1 makes for a very important consideration in this way. Dispersion modelling is another area where accurate equations of state could be deployed with great benefit therefore.

Transportation of carbon dioxide for CCS occurs at high pressures so that more can be transported in a given space of time, and for a lower average cost. It is also the intention that CCS should process only mixtures with the highest possible level of CO_2 , again for financial reasons. If there is to be a leak from the transport vessel therefore, it is probable that high concentration carbon dioxide will be dispersed outwards into a very wide area with very high velocity [47]. A further property of CO_2 is that it is colourless, tasteless and odourless, meaning that it would be very hard to discern whether such a leakage of CO_2 had occurred until the symptoms mentioned above started to set in, by which point it could already be too late. This is especially worrying as carbon dioxide could potentially be leaking for a long time before being noticed and tracked down. Furthermore, with a molecular weight of 44, carbon dioxide is heavier than air, which has an average molecular weight of around 29, and so any such leakage would accumulate at ground level (as opposed to hydrogen or natural gas leakages which would rise away from the ground). The clear safety implication of this is that if there is a carbon dioxide leak from a CCS pipeline close to a populated area, then the humanitarian effect could be disastrous, as it would not disperse from where people are situated, whilst the presence of the carbon dioxide would not be discernible until it was doing harm.

1.3.3 Properties of Carbon Dioxide and its Mixtures

In conducting this literature review, we are frequently reminded of the importance of being able to accurately model the behaviour of CO_2 , both on its own and as part of a mixture. One of the areas of knowledge that is currently lacking, as is evident from the available literature data, is that of thermodynamic pressure–volume–temperature–composition (P – v – T – x) data. This is key in in being able to identify the important features and physical behaviours which need to be accounted

for. Another important consideration for physical behaviour of carbon dioxide is the phase diagram [52], which can be seen in Figure 1.6

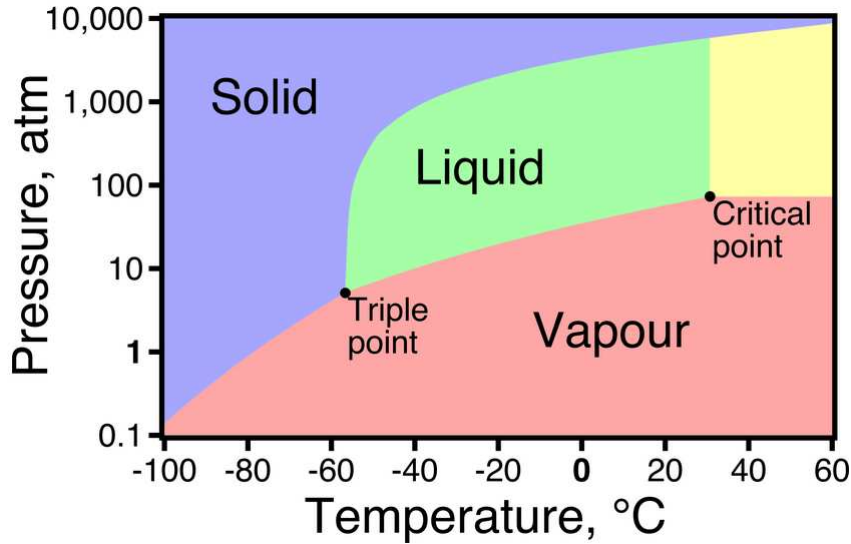


Figure 1.6: Phase diagram for pure carbon dioxide [52]

Both pressure and phase behaviour are important considerations for modelling how carbon dioxide behaves when being transported because the interaction between the liquid and vapour phase determines where the two-phase region lies. There are some density and phase behaviour measurements of carbon dioxide and its mixtures available in the literature, for example [53, 54], although the overall impression gained from such sources is that the data which is available represents a very small amount of that which is needed in order to more fully understand this area [55].

Another important consideration in the modelling of carbon dioxide is its viscosity (see Figure 1.7), which is also calculated by use of an equation of state. Viscosity is the resistance of a fluid to being deformed by a force. Since the carbon dioxide is driven in the pipeline by the high pressure, viscosity is an important consideration as it affects the ability of the mixture to flow more easily, and in turn the energy requirement to drive that mixture. The viscosity of a gas is usually lower than for a liquid of the same chemical species [56].

Also important is the compressibility. Since the carbon dioxide is to be compressed before transportation and subsequent injection and storage, it is advantageous to

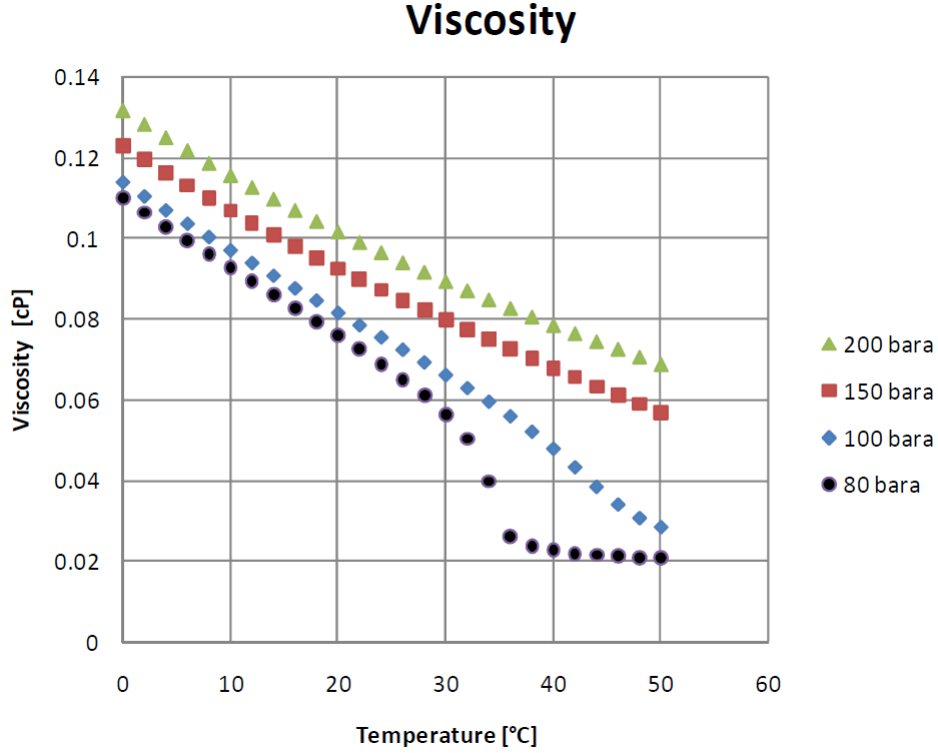


Figure 1.7: Viscosity of pure carbon dioxide as a function of temperature and pressure [56]

be able to do so with the minimum energy penalty, for which an understanding of the pressure behaviour is needed. The compressibility factor Z , defined by

$$Z = \frac{Pv}{RT}, \quad (1.1)$$

where P is the pressure, v is the molar volume, R is the Universal Gas Constant, and T is the absolute temperature. Ideal gases exhibit the property that $Z = 1$, and indeed, setting this in equation (1.1) yields the ideal gas law (IGL). Gases do not usually have this property however, and $Z < 1$ means that the particles can move easily, brought about either by a higher temperature, where the molecules have higher kinetic energy, or by low pressure, in which case they have more freedom to move. In this situation, they can easily be compressed. Conversely, $Z > 1$ means that the molecules have a low mobility, brought about either by low kinetic energy from low temperature, or high pressure. Again, this means that they cannot so easily be compressed. In equation (1.1), the variation of Z with changes in P or T is an interesting problem which gives us some amount of insight to the properties of the substance under consideration [56].

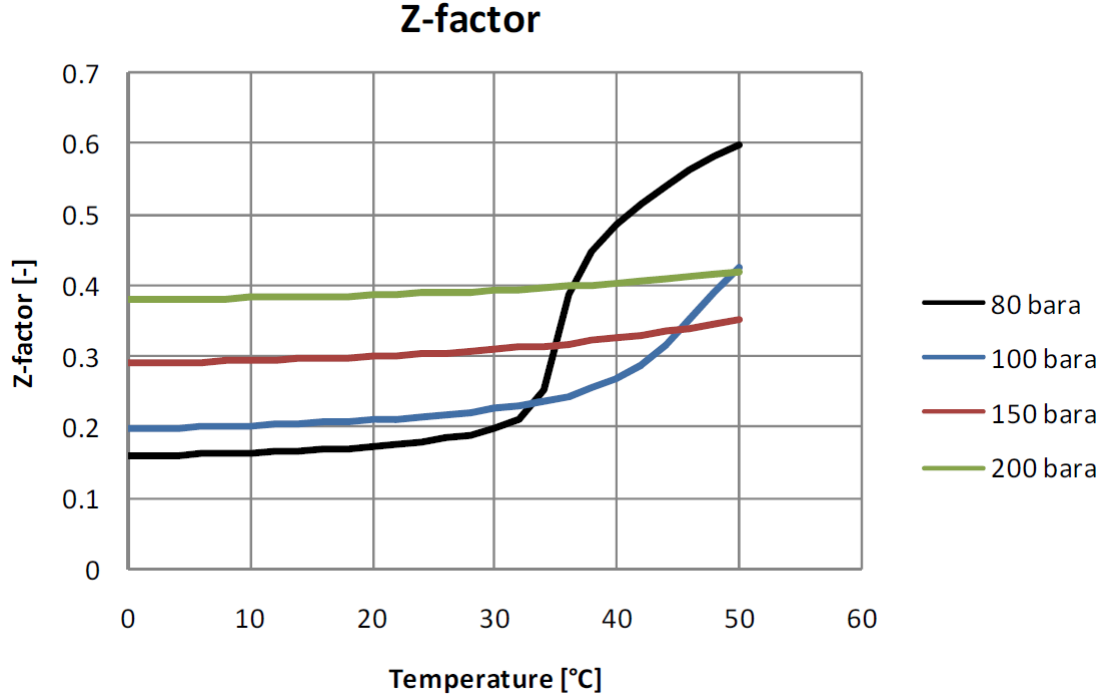


Figure 1.8: Compressibility of pure carbon dioxide as a function of temperature and pressure [56]

Density ρ is also an important consideration:

$$\rho = \frac{m}{V} = \frac{m}{Nv}, \quad (1.2)$$

where m is the total mass of substance being considered, V is the total volume, v the molar volume, and N the number of moles. We note that the quantity m/N represents the molar mass, so by using Equation (1.2) we have a very convenient formulation for relating density and volume. The variation of density with temperature and pressure is also an important consideration when it comes to understanding the behaviour of a fluid [56].

The existence of impurities in the carbon dioxide affects its overall transportability. This is because these impurities affect the physical characteristics such as viscosity, compressibility, density and phase behaviour, as demonstrated in Figures 1.8 and 1.9 [56]. The same qualitative behaviour in changes to viscosity, compressibility and density after the introduction of an amount of impurity are also reported [56], at which point the difference between experimental data and predictions made by an

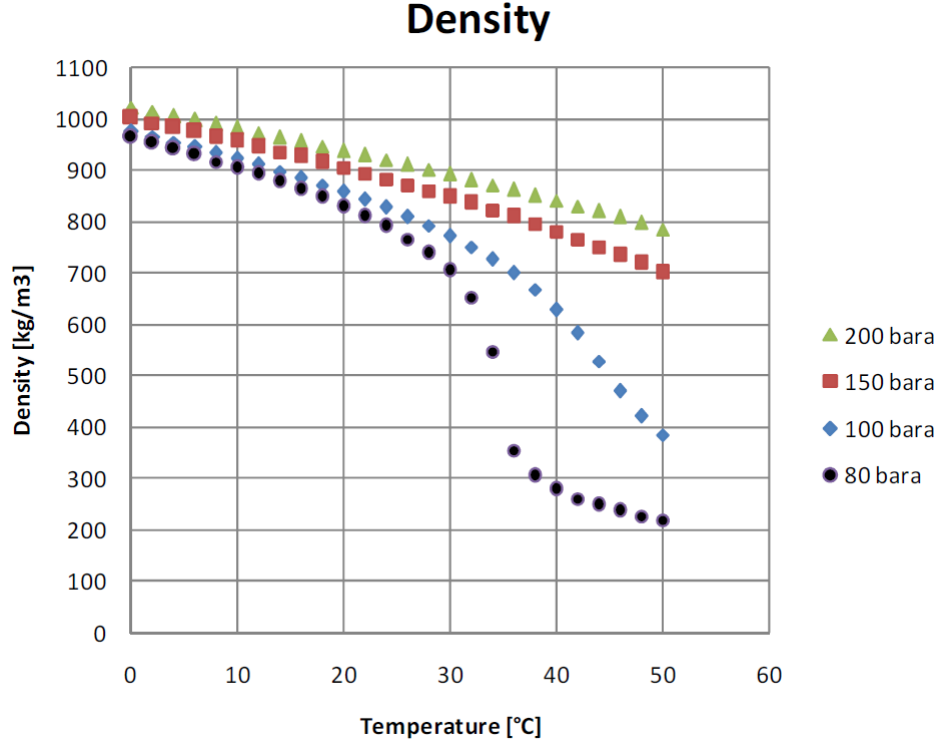


Figure 1.9: Density of pure carbon dioxide as a function of temperature and pressure [56]

equation of state is highlighted. The literature draws on differences between data obtained from ideal theoretical cases and the real practical case [57]. The major disadvantage of depending on experimental measurements of behaviour as opposed to using an equation of state is that these are only valid at the points measured, and cannot usually be interpolated between or extrapolated beyond to give a meaningful insight for any situation not explicitly described. In the field of carbon dioxide transportation, it is hoped that predictive models and equations of state can be backed up by, and used to explain the experimental data, although in some places [57] the literature warns that inefficiencies or inaccuracies of the measuring process could translate into a reliance on poor thermodynamic data.

Because of this, it is not enough to describe a system solely based on experimental measurements. It would seem to be advantageous therefore to incorporate an equation of state when calculating the physical properties, such as the pressure, of a system. Ideally, in order to minimise uncertainty in the description of behaviour of a system, experimental measurements would be validated with an equation. In an area of such uncertainty as CCS transportation, this will be the only way to provide acceptable data, but given there exists such an insufficiency of thermodynamic data

in this area, obtaining a good fit of the relatively few data points which are available by use of an accurate equation of state is highly important.

As has been mentioned in this literature review, it is not expected that CCS pipeline transport will have to deal with a pure stream of carbon dioxide, due to the capture technology used (see Section 1.1.2) and due to the presence of impurities in the fuel itself even before combustion has taken place. In fact, depending on the capture technology used, the amount of chemical impurities can vary, as shown in Table 1.2 [8].

| Capture Technology | N ₂ (% mol) | H ₂ (% mol) | O ₂ (% mol) | SO ₂ (% mol) | NO (% mol) | H ₂ S (% mol) | CO (% mol) | CH ₄ (% mol) |
|--------------------|---------------------------|---------------------------|---------------------------|----------------------------|---------------|-----------------------------|---------------|----------------------------|
| Post-Combustion | Tr. | Tr. | 0.01 | 0.01 | 0.01 | Tr. | Tr. | Tr. |
| Pre-combustion | 0.5 | 1.0 | 0.05 | Tr. | Tr. | 0.05 | 0.05 | 1.0 |
| Oxy-fuel | 2.0 | Tr. | 2.0 | 0.1 | 0.01 | Tr. | Tr. | Tr. |

Table 1.2: Typical dried, treated CCS mixture impurities for different capture technologies

Of course, impurity species are not limited to the most commonly occurring such as N₂, H₂, and O₂, as smaller amounts (on a ppm or ppb scale) of SO_x, NO_x, H₂S, CO, CH₄, and even Hg and Ar, and others can all be present. All of the different impurities can have different effects on the transportability of the carbon dioxide, for example their effects on corrosion or toxicity, which is why it is important to know how much of them is present so that their effect on the physical properties of the carbon dioxide mixture can be calculated by use of an equation of state. It is noted that an ability to factor in the effects of different components on the behaviour of the exhaust stream would be beneficial, and in a way, if such a method that could incorporate any one of the many impurities mentioned here existed, then it wouldn't matter which components were considered in developing this model, as the method would then have scope to incorporate any other compositions at a later date.

Water is usually to be found in significant concentrations in untreated exhaust streams [8], but in light of the fact that this could cause significant corrosion issues, the literature suggests [45, 46] that an extensive drying regime be in place before the transport stage of CCS, bringing this amount down as low as 10ppm, at which point corrosion is no longer an issue. As such, H₂O is not factored into our considerations and figures in Table 1.2 are given for dried mixtures.

A second problem arises from the fact that transportation of the captured CO₂

needs to take place entirely within a single phase, as has been mentioned. When transporting the captured substance (be it in the liquid, vapour or supercritical phase), the pressure drop in the pipeline with distance can be significant (and varies depending on impurity content) [20]. As such, compression pumps are needed at regular intervals: firstly to revive the pressure which drives the fluid down the pipe, and secondly so that the carbon dioxide can be delivered to the injection site at a pressure which is appropriate for that in the storage site. These pumps are highly necessary to the process of CO₂ transportation, and cannot deal with multiple phase mixtures as they need to be set up either to admit a gas, or to admit a liquid, but cannot be utilised to allow both simultaneously. This is due to the differences in viscosities and densities between a gas and a liquid [56] (see Figures 1.7 and 1.9), and is further reason why a clear and accurate identification of the phase boundary is vital. Related to this is the important consideration for how changing pressure can bring about a phase change during pipeline transport. Figure 1.10 shows how different impurities present in carbon dioxide can cause a different pressure drop [20]. The impacts of such a drop are that it affects how often pipe repressurisation is needed, and it could lead to a situation of multi-phase flow if this pressure drop represents a trajectory that would enter the two-phase region.

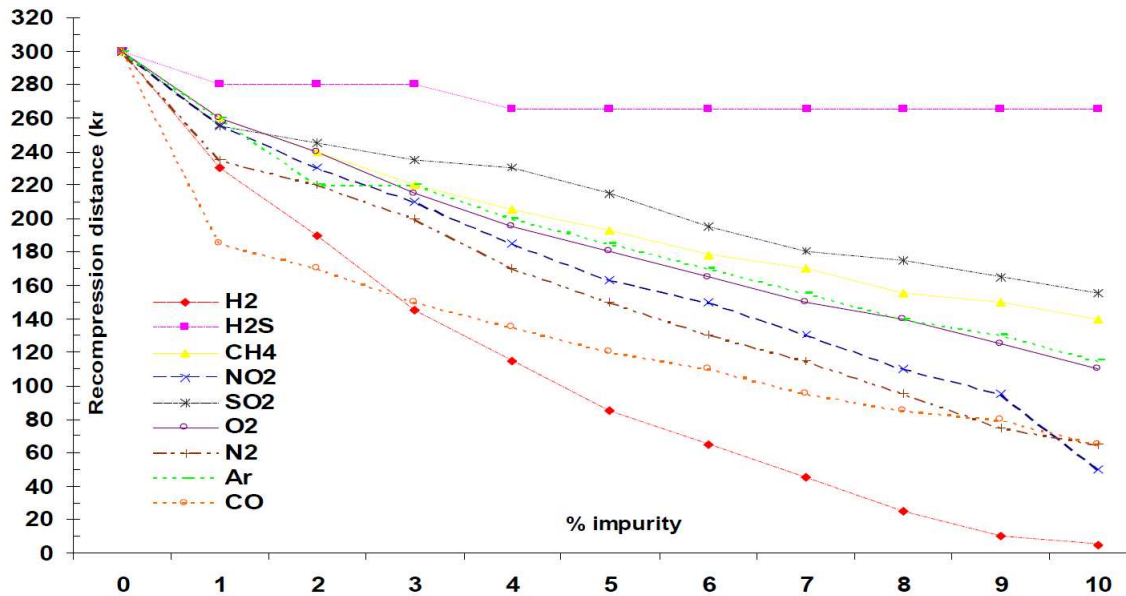


Figure 1.10: Effect of impurity on pressure drop with distance along a pipeline [20]

We can clearly see that the pressure drop with distance is more in the presence of some impurities than others. Also important is how temperature changes with dis-

tance along the pipe, as the evolution of these two variables could determine whether the phase plane trajectory enters the two-phase region mentioned previously. In reality, pipeline transport of carbon dioxide will operate close to the critical point or in the supercritical phase in order to increase density and compressibility and to reduce viscosity, so as to maximise cost-effectiveness. A small fluctuation from the intended operation conditions at this location of the phase diagram could see the mixture enter the multi-phase region. Yet again, this is a clear promotion of the need for an equation of state which is accurate in predicting the phase behaviour of CCS-relevant mixtures.

1.3.4 Pipe Transport of Carbon Dioxide

For the pipeline transportation of carbon dioxide, many lessons may be learned and transferred from the many years of experience in using pipelines to transport natural gas. For CCS, pipe transport is expected to occur mainly in the supercritical region as shown in Figure 1.11 or dense phase region. Here, carbon dioxide exhibits the viscosity of a gas, which is advantageous as this will allow for an easier flow, requiring less of a pressure gradient to drive it, with the density of a liquid, which is again advantageous as it allows a higher mass of carbon dioxide to be transported in any given time. The below diagram shows the location of this ideal operating condition in the phase diagram [52].

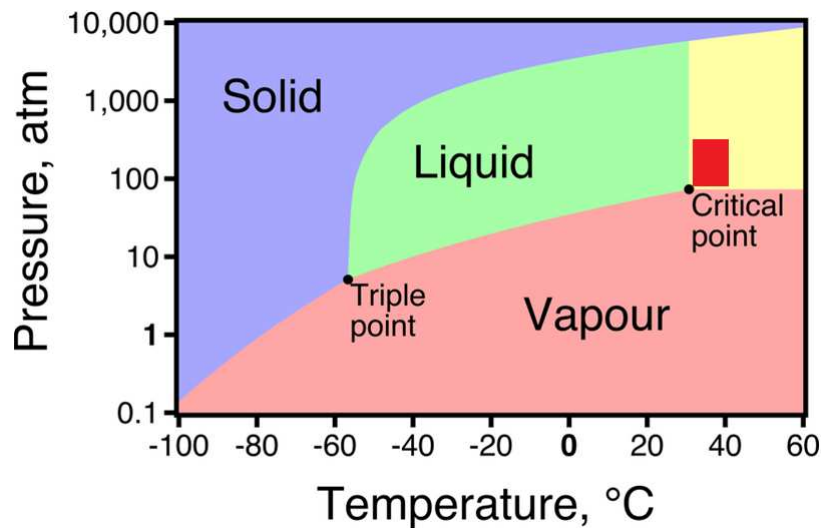


Figure 1.11: Anticipated region of the carbon dioxide phase diagram for pipe transport [52]

The main feature of transportation in this area is not so much the moderately high temperature upto 40°C , but the very high pressure of upto 200bar; or 20MPa. This is important for many reasons, not least because the safety considerations for such high pressure carbon dioxide are significant. The pipeline structure must be capable of withstanding this pressure, as failure at this pressure is likely to cause the dispersion of toxic levels of carbon dioxide over a large area, with the implications as discussed in Section 1.3.2. The necessity of mitigating these risks results in the mandate that pipelines must be very well designed and tested; a process requiring considerable investment. It is estimated that high pressure carbon dioxide pipelines for carbon dioxide transportation will have an installation cost of £1M to 2M per km [51]. With a potential instalment of tens of thousands of km of CCS pipelines by 2050, if CCS is to be successful, this gives a total cost just for the building and installation of these running to tens of billions of pounds, not even accounting for the other four main stages of CCS (see Figure 1.2). This is a massive investment and so the ability to operate safely is even more important. One mitigation strategy for this cost is to have the pipelines running at lower pressures. This causes two problems of its own however, in so far as the final pressure must be consistent with that which is required at the injection site [18], and also that if a lower pressure is permitted in the pipe, then more regular re-pressurisation stations along the length of the pipe will be needed (it may be possible to have CCS pipelines operating wholly in the gas phase). In this scenario, any savings made by running at lower pressure could be countered by the need for a greater number of re-pressurisation stations. The corrosion and hydrate formation considerations mentioned are also important for pipeline transportation. Corrosion must be avoided so as to prevent failure of the pipeline and subsequent dispersion of toxic levels of carbon dioxide. Hydrate formation must be avoided so as to prevent narrowing and blockage of the pipeline which could lead to pressure build-up, culminating in the worst case scenario in a more catastrophic failure. Again, this would lead to dispersion of toxic levels of carbon dioxide. One parameter that can be manipulated to alter the flow rate and thus reduce the likelihood of pipeline blockages is pipeline diameter [58], which also has a profound impact on the running costs of the pipeline. This is something that designers of pipelines could factor into their considerations with the help of a suitably accurate EoS.

As has been mentioned earlier in this literature review, it seems that the preferred option for most of the needs of the CCS transport stage will be pipelines.

1.3.5 Ship Transport of Carbon Dioxide

Ship transportation of carbon dioxide occurs at much lower pressures than in pipelines, close to the triple point of carbon dioxide, for the simple reason that ship hulls are less able to withstand such high pressures. Transportation in the solid phase is impossible due to the lack of fluid properties, and as it would require more energy to get the carbon dioxide onto and off the ship. In order to maximise density (see Figure 1.9), transportation by ship is expected to occur at lower temperature, in the liquid phase close to the triple point [52] (see Figure 1.12).

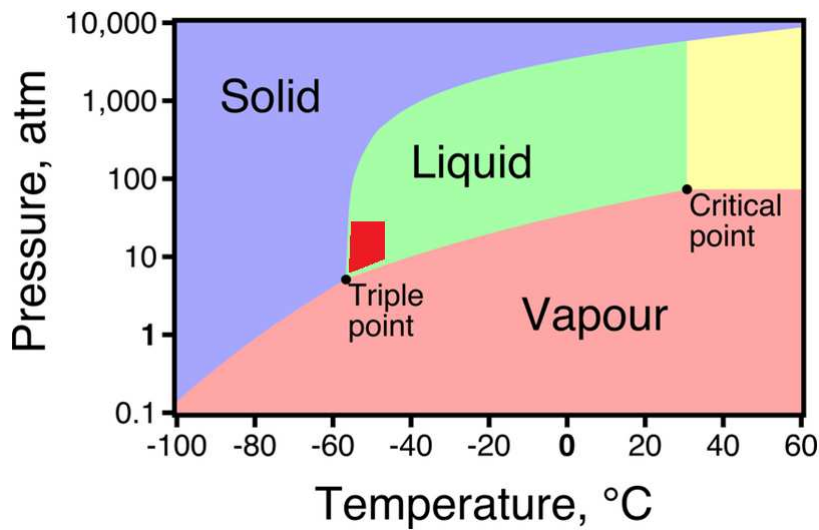


Figure 1.12: Anticipated region of the carbon dioxide phase diagram for ship transport [52]

To be consistent with the aim of keeping transportation costs as low as possible, much of the literature suggests that just as the CCS pipeline transport can take lessons from the EOR industry, CCS ship transport can utilise current knowledge gained from the operation of Liquefied Natural Gas (LNG) transport ships, in terms of dealing with both the pressure and the expected temperature variations. As an example, since carbon dioxide would be transported at around -50°C in ship transport, which is colder than most places on Earth, it is expected that it would heat up during the transportation process. As well as the technical expertise to be gained from LNG transport, it is suggested that combining usage of LNG ships with usage of carbon dioxide ships, by carrying the LNG from ocean to shore in one direction, and both Liquefied Carbon Dioxide (LCO_2) and Liquefied Nitrogen (LIN) from shore to the ocean in the opposite direction as shown in Figure 1.13 [24] would

be an excellent way to minimise the capital costs associated with ship transport [24].

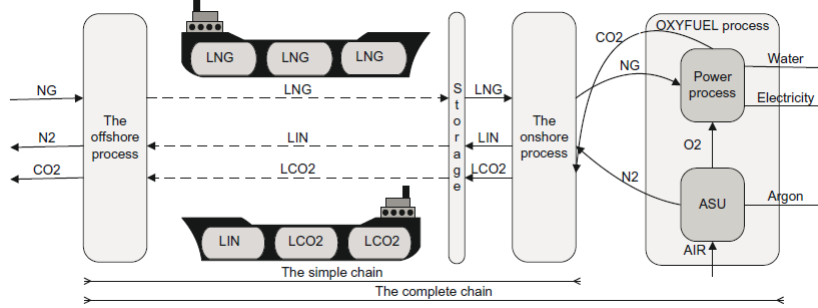


Figure 1.13: Multiple uses of ships to minimise operating costs [24]

One of the main considerations for ship transport that does not apply to pipeline transportation is that the carbon dioxide must be stored prior to loading onto the ship. This causes two problems: if this intermediate storage is at ship pressure, then the storage container must be capable of withstanding this increased pressure, and if not, then there must be enough volumetric capacity to store all the carbon dioxide. As with other factors, this increases both the fixed and variable cost requirements. Despite this, most of the literature [59, 24, 28] seems to be in agreement that over long distances, ship transport offers better cost-effectiveness than pipeline transportation, although this must be offset by the costs of liquefaction, and for shorter distances, pipe transport has the edge.

1.3.6 Compression of Carbon Dioxide

Compression is the stage which comes before transportation in the CCS chain (see Figure 1.2), and the two processes, although technically separate, are inextricably inter-dependent. This is because the pressurisation and the ability to control the pressure at all stages of the transport process is of vital importance. We highlight how important it is to integrate considerations about the operations and limitations of the compression within the transport stage, as well as to highlight how compression, like transportation, has as one of its main aims, the minimisation of its energy requirement, and maximisation of the throughput of carbon dioxide. This brief section is included in this literature review in order to establish the key considerations for this stage of CCS from the point of view of the neighbouring transport stage.

As mentioned, carbon dioxide in CCS must necessarily be compressed in order to

create a driving force within the pipeline and because of the vast amount of it that power generation produces. The extent to which this pressurisation must take place is not without its problems.

All the relevant literature makes some reference to the fact that compression of carbon dioxide is an energy intensive process. We are reminded [19] that in a coal-fired IGCC power plant, compression of carbon dioxide for subsequent transportation can take up more 4% of the gross output of that plant. This represents a large energy penalty. It is also noted [18] that in CCS, there is a target pressure at which the carbon dioxide mixture must be delivered to the injection site. It is mentioned that for most geological sequestration sites, an inlet pressure of around 150bar would be needed [18]. Working backwards along the CCS chain from this, and bearing in mind the expected depressurisation that occurs in the pipeline with distance (see, for example, Figure 1.10), there is a target pressure for the interface between the compression and pipeline transport processes. This cannot be too low as this would result in a lack of drive at the injection site, and it cannot be too high as this would incur unnecessary costs through extra pipe wall thickness, and energy penalties.

Compression systems operate in a multi-stage format, each stage compressing the carbon dioxide a little bit more than the previous, but there are also high-efficiency, single stage compressors [60] currently being developed. These operate by a combination of shock compressors, similar to those used in supersonic flight engines, and the more conventional centrifugal compressor designs. The phase plane trajectory; that is the path taken as temperature and pressure vary is most important during the compression process, just as in the transport process: Depending on the impurities in the carbon dioxide mixture, this can create the scenario of a two-phase region in the phase diagram which must be avoided during compression just as in transport. There are different strategies which can be employed to compress the carbon dioxide from low pressure to high in such a way as to avoid a multi-phase situation, either via a series of small pressurisation and cooling stages, or by one large pressurisation stage followed by one large cooling stage (such as with the shock compressor mentioned above). Yet again, for this task there is a clear need to be able to positively identify both the location of the two phase region and the pressure behaviour depending on impurity [61].

Another important consideration is the quality of the carbon dioxide to be compressed, and for this, it is mentioned that for compression in EOR, a 95% + purity is recommended. For CCS, the required purity will be dependent on the costs as-

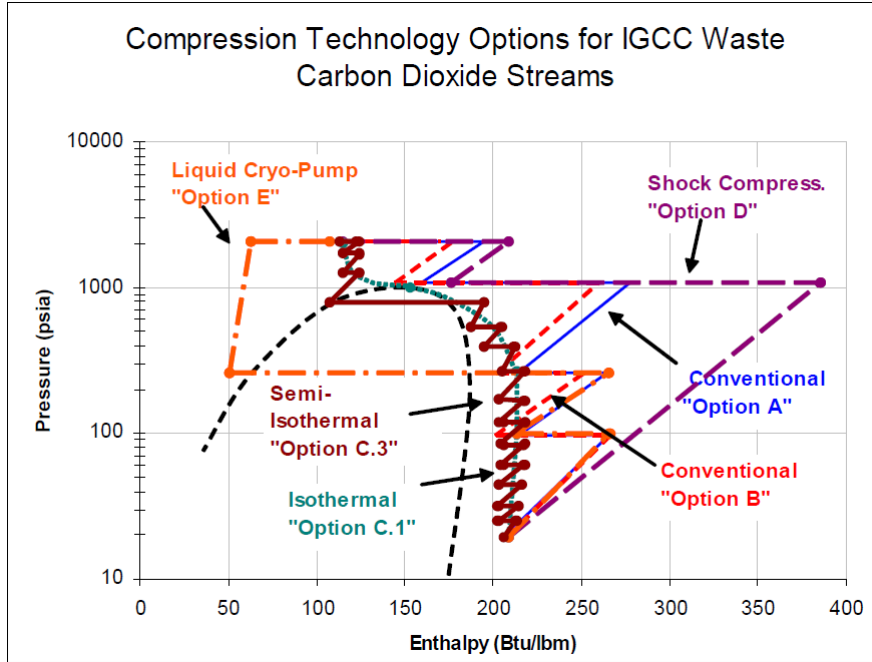


Figure 1.14: Example phase plane trajectories for compression [61]

sociated with transport and injection to the final storage site, but is likely to be higher than this [18, 31]. The fact that the presence of different impurities in differing amounts affects the location of the two-phase region (as is shown in Figure 1.15) causes further issues in this way [62]. Again, this calls out for an equation of state which can accurately predict the exact location of the multi-phase region, depending on the impurities present. In conducting this literature review we found it difficult to find a wide range of data or examples detailing this sort of behaviour other than a few repeated and well-documented cases [62].

As for the energy penalty, once an acceptable compression trajectory has been identified, it is the case that interstage cooling reduces the overall power requirement for CO_2 compression [63]. As for compression methods, there seem to be two main conventional methods which are currently in use; intercooled compression and adiabatic compression with heat recovery [18], as seen in Figure 1.14. Either way, it is noted that the energy penalty in a plant whose output is, for example, 383MW would be around 20MW [18], which is in good agreement with the 4% energy penalty value quoted previously [19]. Traditionally, high-speed reciprocating compressors have been used for CO_2 compression for EOR [64]. This method is more flexible, takes less time, and since the machinery is lighter, can be relocated to a new compression site relatively easily. Some of the literature [64] suggests that in the near future,

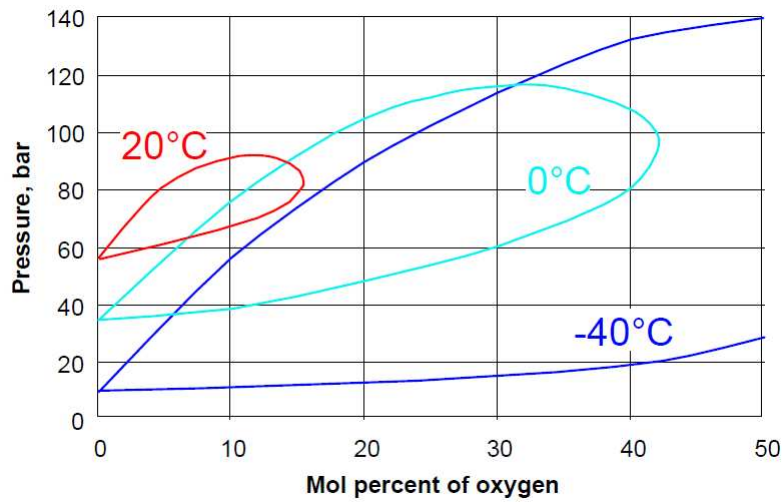


Figure 1.15: Existence of the two-phase region in a carbon dioxide–oxygen mix [62]

centrifugal compressors are likely to be favoured since the capacity of reciprocating compressors would not be large enough to meet the demand for CO_2 compression in CCS. Furthermore, reciprocating compressors are maintenance intensive, and are very expensive to operate. Thus, centrifugal compressors seem to offer many advantages.

The main drawback for centrifugal compressors so far as considerations for the CCS interface with pipeline transport are concerned is that the maximum compression is lower than for reciprocating compressors (see Table 1.3). Nevertheless, since the maximum anticipated operating pressure for CCS pipelines is expected to be around 150–200bar, centrifugal compressors still have the ability to compress the carbon dioxide directly to the required level. There are two main strategies when it comes to CCS compression in anticipation of the subsequent transportation process. Nominally, these are referred to as compression and compression and pumping [18]. Compression and pumping takes into consideration the expected pressure drop during transport. This is an extremely important consideration as the carbon dioxide undergoes significant depressurisation when in the pipeline as shown in Figure 1.10, and so if the injection pressure is to be met whilst also allowing for depressurisation during transit, then either an initial pressurisation to a level far above this is needed, and the CCS pipes must be able to cope with this elevated level, or regular repressurisation whilst the carbon dioxide is in transit is needed. Each option has advantages and disadvantages.

The effect of impurities on the maximum pressure of the pipeline in the case of compression (see Figure 1.10) must therefore be taken into account when determining the pressurisation target for the carbon dioxide, so that it arrives at the storage site at the correct pressure. Again, this demonstrates another application of accurate equations of state. Data, whether empirically or experimentally determined, for the exact depressurisation with distance, depending on a single impurity content has been difficult to find. By way of a summary, we include Table 1.3, extracted from the literature, on the main technologies and performance indicators of existing compression technologies which can be used on carbon dioxide, as a way of highlighting the anticipated pressure ranges equations of state must be applicable to.

| Compression Technology | Maximum Pressurisation (bar) | Maximum Flow Rate (m^3/hr) | Maximum Power (kW) | Source |
|------------------------|------------------------------|--|--------------------|--------|
| Centrifugal | 178 | 82'100 | 11'640 | [63] |
| Reciprocating | 414 | 4'600 | 5'968 | [63] |
| Supersonic | — | 2'621 | — | [60] |

Table 1.3: Existing compression technologies, as summarised from the literature. — means data not available

1.3.7 Regulation, Politics, and Economics

The prospect of transporting high temperature, high pressure carbon dioxide in concentrations which would have toxic effects and could be lethal if leaked, in a vessel constructed of a material which the carbon dioxide mixture could degrade and corrode is understandably unpopular with many people. Moreover, the possibility of external influence on CCS pipelines causing failure and leakage, and the subsequent need for a deep understanding of fracture and dispersion modelling enhances this opinion. The literature goes in to great depth about the many safety requirements that will have to be met to ensure that those who find themselves close to (perhaps within 100m) such transportation networks are sufficiently protected, whilst also avoiding the scenario whereby ensuring this level of safety does not result in such high costs being incurred as to make CCS prohibitively expensive. Of the many important obstacles which must be overcome if carbon dioxide transportation is to be possible, deciding where to place, and how to route the onshore pipelines will prove to be particularly difficult [65, 66], as will trying to convince stakeholders, particularly those who live nearby, of the benefits of placing carbon dioxide pipelines there. To add to the difficulty, obtaining permission from relevant local or national Governments will also be a time consuming and costly process. As an example, since beaches are considered to be areas of natural beauty or of importance to local wildlife, the installation and maintenance of CCS transport infrastructure at coastal

locations is potentially problematic. Listed in the literature are the key stages of proposing a route, assessing the environmental impacts along this route, considering alternative routes and finally obtaining any rights of way for the chosen route [8]. Again, guarantees of safe operation are required.

There are likely to be high levels of inflexibility for the onshore section of the pipeline route as a result: Clearly there is little choice in infrastructure location at either end of the transport process; close to the on-land power plant, and close to the oceanic storage site, but one more also where land becomes sea (this is as true of ship transportation as offshore pipe transportation as there will be similar levels of social resistance to shipping terminals as for pipelines traversing beaches and other sea-side resorts). Of course there may be other points of inflexibility wherever there are areas of dense population, for example in the previously mentioned Humber region of the UK [43]. Furthermore, there will have to be strict regulatory frameworks in place for the injection and storage phases of CCS to ensure that there is no chance of a leak [65]. This highlights another use for accurate equations of state in helping to define pipeline transport purity standards.

Public acceptance of the infrastructure requirements for CCS pipeline transport is key, as it may in some cases be reliant on some fairly irrational fears having to be quelled [8]. The Barendrecht example is important in this regard, as it shows that popular resistance to the idea of CCS-related activities can be enough to stall such projects [67, 27], as demonstrated in Figure 1.16.



Figure 1.16: Popular resistance to the Barendrecht carbon dioxide storage proposals, which eventually derailed the project, including demonstrations (left, [67]) and media hype (right, [27])

As well as resistance from those without technical understanding, a significant amount of resistance can come from those who do understand the technologies and want to raise their own concerns about it through this understanding. As has been

established by this literature review, the pipeline transport of carbon dioxide can be a risky business. A particular issue is energy penalties for the compression and transport processes [68]. Concerns over safety and energy penalties can, in the short-term, only be satisfied by increasing spending, but since CCS is expensive enough already, there will have to be mechanisms in place to ensure that spending on transportation does not get too high. It is the opinion of a selection of CCS experts that the main ways to keep costs low during transportation will be to employ economies of scale and to have fully researched the likely consequences of transport [69].

It is a dangerous position for the implementation of transportation to be in that all three of regulatory, political and economic considerations act as considerable barriers to this being done successfully. This threatens to derail the progress which is being made and so, whereas the implementation of the CCS pipelines is a technical project at heart, it is vital that these considerations are not neglected.

The compression of carbon dioxide to the level required so that it may be transported with the minimum energy penalty through viscosity minimisation and density maximisation requires a very precise knowledge of how the mixture quality affects the thermodynamics of the overall process. This can again be helped by a good equation of state. One of the main criticisms of CCS is that it poses such a large financial cost and energy penalty from capture to storage that left to their own devices, many privately-owned firms would never choose to implement it. This is because the financial penalty brought about by the loss of revenues from power used in CCS instead of being sold to consumers would be too much of a liability.

Very careful management of the operation of capture and transport is needed to minimise the cost burden [70] and the need for Government intervention. The question of how best to minimise the energy requirement to carry out CCS is at the centre of how to implement this process, and herein lies one of the main challenges to be considered; not just in this research project, but by the global energy industry as a whole. Again, equations of state are central to this theme as they will help to define purity standards and develop fracture and propagation models.

The most important fact to remember about transport in CCS is that however large the hurdles to be overcome are, be they social and regulatory [27, 43], financial and economic [69] or technical [68], it is absolutely vital that pipeline transport plays its part or CCS cannot happen. Put simply, this is because if there is no ability to transport the millions of tonnes of carbon dioxide released every year from the

power plants to the geological sequestration sites, and since there is nowhere else to store it, those emissions of carbon dioxide would simply have to be released back into the atmosphere, bringing back into play the environmental concerns raised at the start of Chapter 1.

1.3.8 General Issues Surrounding CCS

As with any technology which promises to radically change established methods of operation, comprehensive risk analyses need to be conducted and safety testing needs to be done, the claims need to be substantiated and economic and financial viability need to be assessed. The first potential problem that arises when one looks at the CCS process from start to finish is that of transporting gas or liquid at high pressure, which has clear safety implications. The materials used to transport matter at such high pressure must have been rigorously tested to ensure that they are up to the task, and contingency plans must be in place, should they fail.

One option likely to be chosen by industry to avoid failures caused by transgressions of small safety margins, is that large safety margins will be put in place for aspects such as the pressures pipes can withstand. This would negate the fact that the exact carbon dioxide mixture behaviour is unknown, but would also constitute potentially unnecessary safety arrangements raising costs even higher. In the scenario of a lack of suitable thermodynamic models, such actions are a likely requirement of government legislation ensuring the new technologies err on the side of caution [48]. As discussed in this literature review, the social implications of placing, for example, a pipeline transporting gas at high pressure through a residential area are unthinkable if the pipe fails (although due to localised social resistances to such a scenario such as seen at Barendrecht, pipeline transportation will generally not be allowed to occur in densely populated areas). A further problem with CCS which is emerging is its interaction with the world of politics and its use as a political tool. The divorce of knowledge and power between engineers and politicians with regard to CCS could result in politically-motivated claims about CCS being made and unobtainable targets for it being set, perhaps resulting in lost confidence in CCS.

For example, the UK Government has pledged an 80% reduction in CO₂ emissions by 2050 [5, 6]. This still seems a very long way off given current trends, and even in the short run, it seems that promises made at the Copenhagen Climate Conference in December 2009 are inconsistent with the aim of global temperature stabilisation [12]. In the long run, this sort of action could lead to a perceived failure of CCS, which could undermine its political viability and subsequent social accep-

tance, including, notably, acceptance for the pipeline transport networks which are so necessary to make CCS happen. The capabilities of CCS therefore need to be clearly defined to avoid this type of misunderstanding. On the theme of political uncertainty regarding CCS, there is also the problem of how all new power plants in the UK are required to be “capture ready” [65]. Although this is so that CCS may be implemented more quickly and easily, the clear problem is that there is no clear definition of what this phrase means, and the potential for ambiguity could lead to a slowdown in deployment of CCS. Indeed, the UK Government has recognised the need to have a definition for what this particular phrase means, and while this definition is likely to take time to be agreed upon, the wider problem of implementing successful capture and transport systems goes on. This, in a sense, encapsulates the regulatory and political problem for CCS, in that it is a time-consuming and bureaucratic process, potentially rife with litigation and delay, whereas the idea of CCS was created because of a lack of available time within which carbon emissions must be reduced.

There are further general problems with CCS. Of these, the organisational commitment required to implement such a large-scale operation, whilst keeping the cost (in both financial and energy terms) as low as possible is particularly prominent. Failure to do so could result in power generation companies concluding that CCS is not financially viable, in which case they could, under a free market system, cease to operate it altogether. This again highlights that economically acceptable operation of CCS is vital, and further promotes the need for an accurate equation of state underlying all considerations for the operation of CCS pipelines.

1.4 A Technical Literature Review

1.4.1 Overview of the Literature Surrounding CCS Pipeline Transport

Having conducted the contextual literature review, we acknowledge the pressing need for an equation of state for application to CCS pipeline transport which is more accurate and more user-friendly than those which are currently available. The main aim of this technical literature review is to advance the ideas set out in the contextual literature review, and to highlight those sources that will be of use to us as we proceed with the technical element of this project.

1.4.2 Physical Constants Used Throughout this Project

We begin by noting some physical constants which will appear repeatedly throughout this work, their numerical values, dimensions, and nomenclature [71].

| Chemical Component | Molecular Mass, M_r (kg.mol ⁻¹) | Critical Temperature, T_c (K) | Critical Pressure, P_c (MPa) | Critical Molar Volume, v_c (m ³ .mol ⁻¹) | Critical Compressibility Factor, Z_c (1) | Acentric Factor, ω (1) | Universal Gas Constant, R (J.mol ⁻¹ .K ⁻¹) |
|--------------------|---|---------------------------------|--------------------------------|---|--|-------------------------------|---|
| Carbon Dioxide | 0.04400964 | 304.1282 | 7.3773 | 9.41185×10^{-5} | 0.274588 | 0.228 | 8.3144621 |
| Nitrogen | 0.02801344 | 126.19 | 3.3978 | 9.01×10^{-5} | 0.291785 | 0.040 | |
| Hydrogen | 0.002015894 | 32.97 | 1.293 | 6.415×10^{-5} | 0.311073 | -0.220 | |
| Oxygen | 0.03199886 | 154.59 | 5.043 | 7.34×10^{-5} | 0.287985 | 0.022 | |

Table 1.4: Values for physical quantities used in this research project. (1) means a dimensionless quantity

1.4.3 The Thermodynamic Basics of Modelling Vapour–Liquid Equilibrium

We note the importance of modelling the interaction between the liquid and vapour phases of a given system within the context of CCS pipelines. In modelling the equilibrium between the vapour and liquid phases within a system, we need to impose [72]:

- **Thermal Equilibrium:** That the temperature within the different phases for each chemical component of the mixture, and between the different components themselves are all the same. We can impose this condition during the modelling of Vapour–Liquid Equilibrium (VLE) by ensuring the same value for the temperature T is used throughout all calculations.
- **Mechanical Equilibrium:** In a similar way to the requirement for constant temperature, we require that the pressure within each phase of each component is matched. We similarly impose this by assuming that the same value of pressure P occurs throughout the system.
- **Equilibrium of Chemical Potential:** That the number of molecules between each phase in each component is not changing, and thus that there are no phase transitions occurring. We do this by matching the fugacity of each phase (vapour and liquid) for each chemical component in the mixture.

If our proposed model is to retain a degree of physical truth, it must be able to compute vapour–liquid equilibrium as well as to give a true relation between volume and pressure. In thermodynamics, generally speaking, an equilibrium can be said to have been reached when the temperature, pressure and chemical potential are all

steady (no time-variation), such as is described in the above list, and that these quantities are matched between distinct phases of a system. For our consideration, this should mean that the numerical value for all of these quantities is the same in both the liquid and the vapour phase for all components in the mixture.

In the case of determining phase equilibrium, an important consideration is the minimisation of the Gibbs Free Energy G . In order to achieve thermodynamic equilibrium, the second law of thermodynamics gives the Gibbs Free Energy G as

$$G = U + VP - TS, \quad (1.3)$$

where U is the system internal energy, V is the total volume, P the pressure, T temperature, and S entropy. Dividing both sides by the number of moles N in the system;

$$\frac{G}{N} = \frac{U}{N} + \frac{VP}{N} - \frac{TS}{N}, \quad (1.4)$$

whence, since the molar Gibbs Free Energy G/N is precisely the chemical potential μ , we have

$$\mu = \frac{U}{N} + \frac{VP}{N} - \frac{TS}{N}. \quad (1.5)$$

In establishing vapour liquid equilibrium, we require that the chemical potential is steady [73], so taking the derivative of both sides of equation (1.5) gives

$$\partial\mu = \frac{1}{N}\partial U + \frac{P}{N}\partial V + \frac{V}{N}\partial P - \frac{T}{N}\partial S - \frac{S}{N}\partial T. \quad (1.6)$$

Since we are seeking the conditions necessary for equilibrium, we may assume that U , P , S and T are fixed (but not V as the volume can change across a phase transition at equilibrium). This leaves

$$\partial\mu = \frac{P}{N}\partial V. \quad (1.7)$$

1.4.4 Fugacity

The Gibbs–Helmholz Equation gives

$$\mu = \mu_0 - RT \log \left(\frac{f(V)}{P(V)} \right), \quad (1.8)$$

where μ_0 is a fixed reference value for the chemical potential and $f(V)$ is the volume-dependent fugacity, with the same units as pressure, exhibiting the property that

$$\lim_{V \rightarrow \infty} f(V) = 0, \quad (1.9)$$

and

$$f(V) = \phi(V)P(V), \quad (1.10)$$

where the dimensionless quantity $\phi(V)$ is called the fugacity coefficient. The concept of fugacity is crucial to modelling vapour liquid equilibrium. It is a quantity which describes a particle's tendency to swap between the vapour and the liquid phases, and so given the original aims for achieving VLE, we note that we should want to arrive in a situation where the values for fugacity at the coexisting points are the same. Differentiating Equation (1.8) gives

$$\partial\mu = -RT\partial\left(\log\left(\frac{f(v)}{P(v)}\right)\right). \quad (1.11)$$

Upon equating the two expressions for $\partial\mu$ in Equations (1.7) and (1.11), we get

$$-RT\partial\left(\log\left(\frac{f(V)}{P(V)}\right)\right) = \frac{P}{N}\partial V, \quad (1.12)$$

whence

$$\partial\left(\log\left(\frac{f(v)}{P(v)}\right)\right) = -\frac{1}{RT}\frac{P}{N}\partial V \quad (1.13)$$

$$= -\frac{1}{RT}\frac{P}{N}\partial V + \left(\frac{\partial V}{V} - \frac{\partial V}{V}\right) \quad (1.14)$$

$$= \frac{1}{RT}\left(\frac{RT}{V} - \frac{P}{N}\right)\partial V - \frac{\partial V}{V}. \quad (1.15)$$

Integrating this over V from V_1 to V_2 and allowing $V_1 \rightarrow \infty$ whilst also setting $V_2 = V$ gives

$$\log(\phi(V)) = \frac{1}{RT} \int_{\hat{V}=\infty}^{\hat{V}=V} \left(\frac{RT}{\hat{V}} - \frac{P}{N}\right) d\hat{V} - \log(V) + \lim_{V \rightarrow \infty} \log(V) \quad (1.16)$$

$$\begin{aligned} &= \frac{1}{RT} \int_{\hat{V}=\infty}^{\hat{V}=V} \left(\frac{RT}{\hat{V}} - \frac{P}{N}\right) d\hat{V} - \log(V) - \log\left(\frac{P}{RT}\right) + \\ &\quad + \log\left(\frac{P}{RT}\right) + \lim_{V \rightarrow \infty} \log(V) \end{aligned} \quad (1.17)$$

$$= \frac{1}{RT} \int_{\hat{V}=\infty}^{\hat{V}=V} \left(\frac{RT}{\hat{V}} - \frac{P}{N}\right) d\hat{V} - \log(Z) + Z - 1 \quad (1.18)$$

where the final terms of the last equality are imposed in order to ensure correct asymptotic behaviour at very low pressures, and where Z is as defined in Equation (1.1). This equation is exactly as given in Equation (2.3.9) of [72] for the fugacity of a pure substance. The implication of the condition that each of temperature, pressure and chemical potential be in equilibrium for substance “ i ” in order for us to determine the VLE is that the value of the quantity $\log(\phi_i(V))$ (with the subscript i denoting the substance) as given in Equation (1.19) be the same at each of the coexisting volumes; the bubble point volume V_{BP} and the dew point volume V_{DP} .

Equation (2.3.1) of [72] also gives the fugacity expression for substance i occurring in a mixture

$$\log(\phi_i(V)) = \frac{1}{RT} \int_{\hat{V}=\infty}^{\hat{V}=V} \left(\frac{RT}{\hat{V}} - \left(\frac{\partial P}{\partial N_i} \right) \right) d\hat{V} - \log(Z), \quad (1.19)$$

which we will also be required to implement in order to impose the correct VLE behaviour of mixtures. We relate Equations (1.18) and (1.19) later.

1.4.5 The Relation Between Volume and Density

We expand Equation (1.2) and note the relation between total volume V with units m^3 , molar volume v with units $\text{m}^3\text{mol}^{-1}$, and density ρ with units $\text{kg}\cdot\text{m}^{-3}$:

$$\rho = \frac{m}{V} = \frac{m}{Nv} = \frac{m/N}{v}, \quad (1.20)$$

where N is the number of moles and m is the total mass in kg. We can immediately identify the quantity m/N in (1.20) as being the molar mass of the substance, values for some substances of which are given in Table 1.4. This convenient relation between molar volume and density means that being able to relate pressure with volume is equivalent to being able to relate pressure with density.

1.4.6 A Summary of Equations of State

As discussed in the contextual literature review, we can see the benefits that might arise if there existed an equation of state which could accurately describe the key physical behaviours of carbon dioxide and CCS-relevant carbon dioxide mixtures. Here we summarise some of the most significant equations of state (judged as such by their overall usage, or contribution to the evolution of equations of state over time). There are many such equations of state available for use in the different stages of CCS. A review of the literature has highlighted the following as being those which

are discussed most often. Here, we discuss the merits and drawbacks of each.

Ideal Gas Law (IGL), 1834

The most basic equation of state combines the general qualitative observations that as the pressure acting on a fluid increases, its volume will decrease, temperature being held constant (Boyle’s Law), and that as the temperature of a fluid increases, its volume will increase, the pressure being held constant (Charles’ Law):

$$P = \frac{RT}{v}, \quad (1.21)$$

where P is the pressure in Pa, T the temperature in K, and $v = V/n$ the molar volume in $\text{m}^3\text{mol}^{-1}$. Here, R is the universal gas constant and has the value as given in Table 1.4. Notice that setting $Z = 1$ in Equation (1.1) yields the IGL (1.21).

The ideal gas law makes a good approximation of the behaviour of many gases in certain circumstances, notably when under low-pressure and the particles are allowed to occupy a large volume, interacting very infrequently. As the pressure is increased however, and these molecular interactions increase, the scope of the IGL to describe how these effect the pressure becomes severely limited.

Van der Waals Equation (VdW), 1873

In order to combat the limitations of the IGL in describing gas behaviour as pressure is increased, the Van der Waals equation was introduced to account for non-ideal behaviour:

$$P = \frac{RT}{v - b} - \frac{a}{v^2}, \quad (1.22)$$

where P , T , v and R have the same units as before, and the quantities a , with units $\text{m}^6\text{mol}^{-2}$, and b , with units $\text{m}^3\text{mol}^{-1}$ are parameters of the equation allowing for an improved flexibility and description of the physical behaviour. The rationale behind this formulation was based on two important theories:

- as the pressure increases and particles move closer together, they are not, in reality, able to get arbitrarily close, as the IGL would suggest. The contemporary understanding of the structure of the atom in the 19th century was such that it was believed that atoms were “hard spheres” (rather like snooker balls), and that they could not be deformed or compressed beyond the limits of their boundaries. Thus, upon increasing the pressure to arbitrarily high values, it would not be the case that atoms could get infinitely close together,

but instead could never approach closer to each other than the diameter of one of these hard spheres (using the snooker balls analogy again, this would be equivalent to noticing that you could only ever fit n balls into a box designed to accommodate n balls, no matter how hard you try). This therefore excluded an amount of volume from the consideration, so the term containing b in the VdWEoS is often referred to as the volume exclusion term. Whereas the hard spheres interpretation of atomic structure is now known to be invalid, the volume exclusion term still retains a significant amount of physical relevance at all but the most extreme of pressures.

- there are other important physical interactions that exist between particles, notably that forces created by charge come into play at small distances. In the 19th century it had been understood for some time that protons and electrons carried opposing charges (neutrons had not been identified yet). Under the hard spheres interpretation of the atom, it was believed that the negatively charged electrons sat on the surface of the sphere, which contained the positively charged protons. As atoms came into close proximity, the opposing charges caused an attractive force. This effect is described by the parameter a , and the term containing this parameter is referred to as the attractive potential term.

The Van der Waals equation represented a step forward in thinking about describing physical behaviour of fluids, but ultimately it still falls some way short in accurately describing this.

Redlich–Kwong Equation (RK), 1948

The Redlich–Kwong EoS [33] extended this thinking by elaborating on the VdWEoS. They suggested

$$P = \frac{RT}{v - b} - \frac{a}{\sqrt{T}v(v + b)}, \quad (1.23)$$

with all quantities having the same dimensions as before. By doing so, the aim was to give the model more flexibility in describing complicated physical behaviour. The parameters a and b were defined:

$$a = 0.4278 \frac{R^2 T_c^{5/2}}{P_c} \quad (1.24)$$

$$b = 0.0867 \frac{RT_c}{P_c} \quad (1.25)$$

In the paper in which Redlich and Kwong proposed this equation, the importance of calculating fugacities was also acknowledged. As we have seen from Equation (1.19), fugacity is a vital concept in modelling VLE.

Soave–Redlich–Kwong Equation (SRK), 1972

The Soave–Redlich–Kwong EoS is another cubic equation state, further developing the previous models.

$$P = \frac{RT}{v - b} - \frac{a}{v(v + b)}, \quad (1.26)$$

with all quantities having the same dimensions as previously, but with parameter definitions altered slightly:

$$a = 0.42748[1 + (0.48 + 1.574\omega - 0.176\omega^2)(1 - \sqrt{\frac{T}{T_c}})]^2 \frac{R^2 T_c^2}{P_c}, \quad (1.27)$$

$$b = 0.08664 \frac{RT_c}{P_c}. \quad (1.28)$$

The Soave–Redlich–Kwong was a modification to the previous version of the model, incorporating for the first time a consideration for the effects of the relative distribution of mass and charge in different chemical species which would have an effect on physical behaviour, the parameter describing this being ω , and being referred to as the acentric factor.

Peng–Robinson Equation (PR), 1976

The Peng–Robinson equation [34] of state also incorporated use of the acentric factor:

$$P = \frac{RT}{v - b} - \frac{a}{v(v + b) + b(v - b)}, \quad (1.29)$$

where the quantities again have the same dimensions as before, and parameters this time being defined as

$$a = 0.45724[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{\frac{T}{T_c}})]^2 \frac{R^2 T_c^2}{P_c}, \quad (1.30)$$

$$b = 0.07780 \frac{RT_c}{P_c}. \quad (1.31)$$

It is noticeable that the PREoS took an almost identical form to that of the SRKEoS, suggesting that it had been the intentions of the creators not to generate a new form

of equation, but to seek an improvement to an existing equation through numerical optimisation. This is a key concept in the evolution of Equations of State.

Span–Wagner Equation (SW), 1996

Whereas the above equations of state all belong to the family of cubic equations, the Span–Wagner equation of state is a completely different type. It is of far higher order, and is calibrated with a high number of parameters, thus giving it exceptional performance. Typically this is less than 1% out [74] from established experimental data, but the usual accuracy of the Span–Wagner equation in describing the key physical behaviour of pure carbon dioxide makes it a good substitute for having the experimental data, and often this equation is taken to be the authority on describing pure CO₂. The major drawback of the SWEoS which precludes it from being of any value in CCS despite its tremendous accuracy is its inability to describe anything other than pure carbon dioxide.

Wide–Range Equation of State for Natural Gases and Other Mixtures (GERG), 2008

The GERG is similar to the SWEoS in that it is highly parametrised and of high order, exhibiting a high degree of accuracy in most cases, and for most CCS–relevant chemical species including hydrogen. It is very often referred to in CCS documentation as giving excellent descriptions of the physical behaviour of many CO₂–rich mixtures, except notably in the case of binary mixtures of carbon dioxide and hydrogen. The major limitation of the GERG is its computational complexity, which in a similar way to the SWEoS may prohibit it from a wider deployment in helping to understand CCS pipeline transport. In the case of pure CO₂ the GERG equation is the same as SWEoS. There is a previous version of the GERG, from 2004.

Relative Performance of Existing Equations of State

The literature makes reference to all these equations to varying degrees. We found the model referred to most often in the literature and discussed at conferences was the PREoS, for its relative ease of use and computational simplicity. This is in spite of its disability in describing certain behaviours which are key to the understanding of CCS pipeline transport, most notably the trouble it has in dealing with liquid–incompressibility and mixtures, where its errors can reach 40% (see Table 4.2), even in the pure case. We felt, as is echoed by many in the CCS industry, that this sort of performance will not be suitable for use in helping to accurately predict the behaviour of the gas in the pipelines, due to the implications discussed in Section

1.3 of this thesis.

The next most commonly mentioned model was the GERG, often cited as being of great use in describing the VLE of CO₂-rich mixtures for all CCS relevant chemical impurities apart from hydrogen. Typically errors were around the 1-3% mark, which we suggest would be acceptable for use in CCS.

The SWEoS is often held up as an example of what CO₂ equations of state could achieve if it could be generalised to other chemical components, but ultimately, this drawback is its downfall, and is why it too is unsuitable for use in CCS. Despite this, it does highlight that tremendous accuracy can be achieved in an EoS by utilising a very high number of parameters (188 in all in the case of the SWEoS), whereas we should not be surprised to find that the PREoS with only two fitting parameters can struggle to explain the data. We also note however that the size of the window of relevance also plays a role in the trade-off between simplicity and accuracy, and that an equation which aims to describe physical behaviour over a very wide range is bound to suffer from lower accuracy or the need for increased complexity. An equation which was specifically focussed on the temperature and pressure window of operation for CCS pipelines could potentially exhibit a level of accuracy as needed for application to CCS pipelines without a requirement for extra terms or model parameters.

1.4.7 A Summary of Literature Thermodynamic Data Used for Fitting

As part of the technical literature review, we conducted an extensive review of the available thermodynamic data from various literature going back as far as 1930. This was because we would need to fit any proposed equation to the physical data. We summarised this data from the literature in the Appendices either into the form $P-v_{BP}-v_{DP}-T-x-y$ if being used for VLE descriptions, or $P-v-T-x-y$ (we use x to denote the concentration in a liquid and y to denote the concentration in a vapour) if being used for density-pressure descriptions. It was further sub-categorised into sections pertaining to the particular binary mixture which was being described.

As was highlighted by Table 1.2, we determined that the most commonly occurring impurities to be found in CCS pipelines were nitrogen, hydrogen, and oxygen, after water had been removed due to its role in causing corrosion. We thus summarised data for binary mixtures CO₂-N₂, CO₂-H₂, and CO₂-O₂. We note at this point the almost total lack of ternary data for any of the derivative systems of these

mixtures which contained mostly carbon dioxide. Where the literature data had been given in units other than S.I. (MPa for pressure, $\text{m}^3\cdot\text{mol}^{-1}$ for molar volume, K for temperature), we manipulated it from its published form into these standard units in order to make for an easy application to our method.

As was to be expected, the literature data was presented in a very wide variety of formats (isothermal, isobaric, isochoric), and so had either to be analysed and converted into a form we could use, or discarded. Since many equations of state such as PREoS give a formulation for the pressure in terms of volume and temperature $P(v, T)$, and given the volume-dependent nature of the necessary fugacity constraints (1.19) and (1.16) which we would have to impose during model development, we highlight here the necessary criteria for the data to be of use to us in our fitting:

- The data must contain the full array of thermodynamic information. That is pressure, molar volume, temperature, and composition (such data being henceforth referred to as P – v – T – x data), or information allowing us to formulate this array. For example we could calculate molar volume v from the compressibility factor Z (see Equation (1.1)) or from density ρ (see Equation (1.2)).
- The data must be isothermal.
- For VLE data, this must be given at coexisting pressure and not coexisting composition.
- Since an equation of state should be able to give predictions for both density–pressure and VLE behaviour, it will be useful if we could find both these types of data at each temperature, although not essential, because to a certain degree the density behaviour can be inferred from VLE data.

The data we collected from the literature is summarised in the Appendices. We also acknowledge the National Institute of Standards and Technology database [74], from which we could take the required thermodynamic data for pure substances.

1.5 Project Aims

1.5.1 Motivation for this EngD Research Project

CCS is one of the main medium–to–long term strategies by which it is hoped the environmental impact of power generation and other heavy industry can be minimised.

It is evident from this literature review that the role of transport in CCS is vital. Furthermore, the ability to safely carry out the transportation of carbon dioxide for CCS is highly dependent on both the impurities that reside within it from the fuel that was used in combustion, and the capture process itself. This necessitates an equation of state which is specific to this particular cause.

A crucial and often overlooked aspect of the CCS chain is CO₂ transportation, for which technological and legislative issues on how to transport large volumes of CO₂ in a safe and energy efficient manner remain. Whilst CO₂ pipelines have been operational for over 30 years, mainly in the United States for EOR, transportation of anthropogenic CO₂ on the scale required for CCS has not been attempted before [41]. Again, a suitable equation of state would help to implement this with increased certainty of safety and success.

Following on from our analysis of the various equations of state available at present, and in light of this need, we feel therefore that there is a pressing need for a new equation of state for a specific application to the design and operation of CCS pipelines, which is simultaneously both sufficiently user-friendly and accurate.

1.5.2 Formalisation of Aims

This main aim of this EngD project shall therefore be to propose a new equation of state which is particularly relevant to CCS pipeline transportation. Specifically, we will aim for it to be highly accurate within the expected window of mechanical and thermal operation of CCS pipelines; upto 200 bar and between approximately 0 and 40°C. It would also be useful for dispersion modelling if the accuracy of the model could last down as low as approximately -10°

We will aim to define the new equation of state in the form $P(v, T)$, so that it can easily be used for describing the key physical behaviours of CO₂ such as density-pressure relations, as well as phase behaviour during the pipeline transport stage of CCS. It is our intention that this equation should simultaneously be more user-friendly than some other EoSs, which can be very complicated, and which do not generalise to the case of mixtures, whilst also being more accurate than those which are currently widely used.

Taking as inspiration the performance of currently available equations, we feel that if we could demonstrate that our equation can have an inaccuracy level of under 2% for descriptions of pure carbon dioxide, and under 5% for mixtures in both VLE

and density predictions, whilst also retaining a suitable level of simplicity, this would represent a significant improvement over the currently widely used models. In order to position our equation thus, we observe the evolution in the form of these currently used equations of state from the simple, such as the IGL, VdWEoS, RKEoS, SRKEoS and PREoS through to the more complicated such as the SWEoS and GERG, and note that although the PREoS is widely used due to its simplicity, it is unsuitable for describing CO₂ behaviour in CCS transport due to its consistent lack of accuracy throughout the region of interest, exhibiting errors as high as 40% in some places, and that whereas the SWEoS is highly accurate, this comes at the cost of a very high degree of functional complexity and a reliance on a large number of parameters, making it very difficult to work with and generalise to the case of mixtures. This suggests we should look for something between the PREoS and the SWEoS in terms of both complexity and accuracy.

To bring about this aim, we will thus seek an equation that would match the literature experimental data or data taken from NIST significantly more accurately than the PREoS, but without the need for high functional complexity, or the requirement for a large number of parameters predominant in more complicated equations of state, although we do note that for descriptions of pure CO₂, NIST uses the SWEoS due to its superior accuracy in this case. This data is generally not more than 0.05% out from peer-reviewed experimental data, making it ideal for our purpose of being highly accurate data to which we will fit our equation in the case of pure carbon dioxide.

1.5.3 Scope for Application of this Project

One of the main barriers to overcoming the many political, social and regulatory issues surrounding CCS transport is our current lack of ability to predict how the physical properties of carbon dioxide change as the type and amount of constituent chemical impurities vary. Presently, there are several equations of state which could be utilised, but all have their relative drawbacks. Bearing in mind there is a balance to be struck between faster equations and those which are more accurate, then in particular, there is a clear need at this moment for the development of an equation of state which can accurately depict the physical behaviour of carbon dioxide and impurities during the transport stage of CCS in a simple, effective way without excessive computational cost.

There is also much that needs to be better understood before safe, socially acceptable and cost effective transport networks can be constructed, especially in the

prediction of key physical behaviour such as density–pressure or volume–pressure and phase behaviour. We feel that if we are able to formulate the model specified within our aims in Section 1.5.2, this will be of tremendous value in the design and subsequent operation of CCS pipelines, and in this way will have a very clear application and hopefully, a large demand.

Chapter 2

Methodologies and Mathematical Techniques to be Used in this Project

2.1 Outline of Method

Following on from the literature review and project aims set out in Chapter 1, we will proceed by proposing a physically relevant formulation for our equation of state. Based upon our observations made in the literature review of the natural trade-off between the complexity and performance of an equation, we will be required to ensure that our proposed model has sufficient flexibility to obtain the target level of accuracy outlined for the proposed model. If this target can be achieved in the majority of cases, we will deem the project to be a success, as we will feel a very good compromise between the the simpler, less accurate equations, and those which are more complex but also more accurate would have been found. In doing this, we feel we will have offered a very tangible solution to many of the design and operation problems CCS pipeline transport faces due to a lack of certainty in the prediction of physical behaviours.

Like those equations such as the PREoS at the simpler end of the spectrum, we will make ours pressure-explicit, and it will be given as a function of the temperature T and the molar volume v , as is also the case for the PREoS; one of its features which makes it particularly user-friendly. It will also depend explicitly on

a number of parameters; quantities which we will be required to give temperature dependent definitions for in order to allow our model to render full thermodynamic descriptions of density and phase behaviour. Thus, the equation will be of the form $P(v, T; a, b, c, \dots)$, where a , b , and so on are the parameters of the equation, and the “...” is used to denote that the pressure depends on as many such parameters as we feel is necessary to give the model a good chance of being suitably accurate. This will be a two-stage process:

Firstly, we will fit the equation to the pure CO₂ data taken from the NIST database [74] in order to give temperature-dependent expressions $a(T)$, $b(T)$, ... for each of the model parameters. The temperature range of these expressions will be the same as the CCS-relevant window of temperatures, which the literature review and attendance at many conferences suggested as being similar to atmospheric temperatures for the majority of planet Earth, around 0 to 40°C. The pressure range will be from atmospheric pressure up to 200bar, which we understand to be approximately the necessary maximum in order to maximise throughput whilst limiting the financial burden, as noted in Table 1.3. In the first instance, this will have created an equation of state which is valid in the case of pure carbon dioxide only, in the region of interest of CCS transport, and this will then form the foundation of the rest of the model.

We will subsequently consider binary mixtures, and for each distinct mixture highlighted as being of particular relevance to CCS in Table 1.2, we will propose mixing rules for each of the parameters from the original equation to allow this generalisation. At this early stage, we acknowledge, based the role played by parameter a in the PREoS, that linear mixing rules may not be sufficient to allow a suitable degree of flexibility in the fitting, and we are prepared to have to try quadratic mixing rules as necessary. The literature review revealed that the most consistently occurring chemical impurities likely to have a major impact on the pipeline transport of CCS are nitrogen, due to its abundance in the atmosphere and subsequently in CCS mixtures, hydrogen, emanating from combustion of the fossil fuel, for which an interesting point is that even the GERG is acknowledged to have some shortcomings, and oxygen, also naturally occurring in the air and used for the combustion of the fossil fuel, occurring in significant quantities in CCS. Since drying regimes will be very strict in order to minimise pipeline corrosion, we do not incorporate water into our consideration for the model.

An important realisation is that the mixing rules for each parameter will themselves be dependent on sub-parameters, which we will also need to find temperature-dependent expressions for. This will be done following on from our extensive har-

vesting of data from the literature, we will use that which we deem appropriate to calibrate the proposed system; which incorporates both the original equation, and the mixing rules. For nitrogen, hydrogen and oxygen in turn, we will load the literature and NIST data, formatted into “.txt” files, either sub-categorised into density or VLE data, to our chosen modelling software package “Mathematica 9 for Students”, by Wolfram. From here, we will write code and algorithms to utilise the software in minimising an error function for the sub-parameters, ensuring both density and phase behaviour is adhered to, and in doing so, we will be able to determine the numerical value of each parameter at the temperature we fitted to the data at.

This will be repeated at each temperature point within the CCS-relevant temperature range we have been able to collect data for until we are able to specify the value of each parameter at a variety of temperature points throughout this range. We will subsequently give a temperature-dependent form for each of the sub-parameters, thus closing off the system and allowing us to give a formulation for P solely in terms of v and T for each binary mixture..

2.2 Selection of Data

Before proceeding to fitting the proposed equation to the various NIST and experimental data we collected, a thorough survey of available density and coexistence data sets was conducted. This utilised various other literature reviews done previously [55, 75] as well as other data sets found manually by searching through on-line journals.

As mentioned in the introductory chapter, in order for our method to be able to utilise a particular data set, we required the following:

1. In the case of homogeneous density data, the set should contain the full array of thermodynamic information: the pressure P , the molar volume v , the temperature T , and the composition of the mixture x . Alternatively, it could give values that would allow a direct calculation of these four variables, for example, v could be calculated from Z by use of equation (1.1), or from ρ by use of equation (1.20).
2. In the case of coexistence data, that coexisting dew and bubble points be given at constant pressure as opposed to constant composition. Thus, we need each data point in the form $P-v_{BP}-v_{DP}-T-x-y$, where v_{BP} is the bubble point molar volume and v_{DP} is the dew point molar volume.

3. Ideally, that the data be precisely isothermal, or alternatively not more than a few thousandths of a Kelvin out from each other at each data point, in which case the data would be considered isothermal.

Based on the accumulation and subsequent analysis of the literature thermodynamic data, we made the following observations:

1. A lot of the data was incomplete in respect of either point 1 or 2 above. In our reproduction of thermodynamic data from the literature in the Appendices, we used “ — ” to denote a piece of data which was not available. It can be seen that this occurred very regularly within the literature.
2. Specifically, the majority of the surveyed VLE literature contained neither any reference to the molar volumes, nor any data allowing us to calculate these (compressibilities or densities). Our initial approach had been to abandon such data and only consider using the data which gave all values P – v – T – x , but upon a holistic analysis of the data we concluded that this would have resulted in us discarding the vast majority of the VLE data, to the extent that we would not have been able to carry out a fitting with the data that was left. As a direct result, after considering estimating these through either Maximum Likelihood Estimation or as part of the numerical search algorithm, we produced a novel non-probabilistic estimative method for reconstructing these missing volumes, so that the majority of the data could be salvaged and utilised in the fitting.
3. Some sources [76, 77, 78] listed their measurements in ways other than isothermally. Where such data could be reconfigured into such a form that rendered it isothermal, we did this, otherwise we discarded it.
4. At some points the compositions were not reported. In this case we had to discard that particular data point.
5. Occasionally [79] some sources plotted the data in graphical form but did not seem to include the tabulated data. In this scenario we also had to neglect that data.
6. Some of the data we summarised was at a temperature far outside the range of relevance for CCS pipeline operation. This was discarded. For example, in [80], the temperatures (543–704K) were too high. Similarly for [81] (673.15K).
7. Occasionally, published data was not isothermal, in this case usually being isochoric [82], or occasionally at constant composition [75]. In particular,

some of the data presented in [82] was isochoric, and some approximately isothermal. The isochoric data was discarded.

8. We found some contradictory data, as is to be expected in a data survey as comprehensive as that which was undertaken here. This is even less surprising, given the data was measured across a period of many years, different institutions, and using a wide variety of methods, for example by use of a Pycnometer or Burnett Apparatus for density measurements.
9. A lot of sources listed virial or calculated/optimised binary interaction coefficients [83, 75, 84, 85] based on work they had done. We did not concern ourselves with those as our aim was to fit a completely new equation of state rather than to optimise existing equations.
10. The given values for critical properties seemed to be inconsistent between sources, e.g. in [75] where a value for the critical pressure of carbon dioxide of 7.3752MPa was taken; a slight disagreement from the figure we used based on the majority of other sources, as detailed in Table 1.4.
11. Some data appears to have been duplicated within the literature [83, 86]. In this case several of the authors of both papers were the same.
12. Some sources gave measurements for pure components, for example for pure carbon dioxide [87, 88] or pure nitrogen [89]. The conclusions drawn in these sources suggested that the methods they had used to generate their data were consistent with the Span–Wagner equation in the case of pure carbon dioxide. Thus, owing to the superior availability of data and similar accuracy, we opted to take all our pure data from the NIST database.
13. There was an abundance of density measurements for the binary system CO_2 – CH_4 [53], but very little by way of VLE data, and that which was available was very fragmented, meaning it would have been difficult to include considerations for CH_4 at this stage.
14. The VLE data reported in [53] was not given at constant vapour pressure, as required by our method, rather it was given at coexisting compositions. We thus used a smoothed linear interpolation on their reported pressures to allow us to use this data as the lack of any other sources for this composition coupled with the comprehensive nature of this particular data set required us to do so.
15. Very infrequently [90, 91] some data was found to be extremely lacking in quality. In such cases, the lack of internal consistency was exposed by our equation

when we tried to fit using it. In this case we neglected the volume element of these measurements and employed our own volume estimation method.

2.3 Availability and Coherence of Data

Generally, we found the availability of data detailing both homogeneous density and VLE behaviour at the same temperature to be low. Furthermore, that which was presented was done so in a wide variety of formats, in different units, and with some elements missing. In the literature review, much was made of the lack of high-quality thermodynamic measurements which are of relevance to the CCS pipeline transport industry, and given that the calibration of any relevant equation of state, including our own, is dependent on the availability of such data, we include in our conclusions suggestions for which measurements can be taken next in order to allow for this to be done.

We carried out a brief analysis of the state of the literature data in its current form, and found that all the given pressure–density measurements could be used, as these always contained the information we required. For the VLE data it was a different story however and much of it would have had to have been discarded unless we could incorporate a good estimate for the volume values it was missing. the extent to which we would have had to discard large amounts of data without this estimation method is shown in Table 2.1.

| Mixture | Usability of data? | | | Total |
|---------------------------------|--------------------|------------------------|-------------|-------|
| | Yes | With Volume Estimation | No | |
| CO ₂ –N ₂ | 40 | 239 | 123 | 402 |
| CO ₂ –H ₂ | 0 | 185 | 131 | 316 |
| CO ₂ –O ₂ | 26 | 109 | 134 | 269 |
| TOTAL | 66 (6.7%) | 533 (54.0%) | 388 (39.3%) | 987 |

Table 2.1: A summary of the number of literature VLE data points needing to undergo volume estimation in order to be used in fitting

Without a method for utilising the data where volumes are missing, we would only have been able to use 6.7% of the literature data. With volume estimation, we were in a position to use up to 60.7% of that data, thus giving the equation more physical relevance.

2.4 Estimation of Coexisting Molar Volumes

As noted previously, we observed that a lot of the VLE data, especially that describing the binary systems $\text{CO}_2\text{--H}_2$ and $\text{CO}_2\text{--O}_2$, found in the literature was lacking a volumetric element. Such data points are noted in the Appendices under the “Vol. Est.” column, by which we meant that even though the data point did not contain the volumetric information, it might be still be usable if we could somehow introduce a suitable method of volume estimation. We thus developed from scratch a novel process to estimate both the bubble and dew coexistence volumes in compensation for those data missing in the literature. This was primarily down to the fact that our method of fitting the parameters to the chosen form of the equation required all elements of the thermodynamic description (temperature, pressure, volumes and compositions) to be present, but owing to the relative sparsity of VLE data containing all this necessary information (see analysis in Table 2.1), we felt some way of incorporating that which was available would be better than discarding it altogether. We do, of course, acknowledge that experimental measurements of a quality high enough to be published in peer-reviewed journals would have been preferable to having to estimate volumes.

2.4.1 Mixture Bubble Point Volume Estimation

In the following two Sections we denote a bubble point volume by u and a dew volume with w for notational convenience.

We estimated the mixture bubble volume \tilde{u}_{MIX} by taking a weighted average of the pure carbon dioxide bubble volume and the pure nitrogen (respectively, hydrogen, oxygen) volume at the same pressure, with the weighting given by the concentration of nitrogen (respectively, hydrogen, oxygen), adjusted by an empirical constant ξ_{BP} . The pure data was available in all cases from NIST, and the compositions were reported as part of the literature data. This definition was given for each temperature and pressure by:

$$\tilde{u}_{\text{MIX}} := (1 - x_{\text{N}_2}^{\xi_{\text{BP}}})v_{\text{CO}_2} + x_{\text{N}_2}^{\xi_{\text{BP}}}v_{\text{N}_2}, \quad (2.1)$$

where \tilde{u}_{MIX} is the estimated bubble volume of the mixture at the required temperature and pressure, x_{N_2} is the concentration of nitrogen at the bubble point as quoted in the literature, v_{CO_2} is the molar volume of pure carbon dioxide at this temperature and pressure, v_{N_2} is the molar volume of pure nitrogen at this temperature and pressure, and ξ_{BP} is a novel, empirically determined constant included in order to calibrate this estimation for different mixtures. This dimensionless quantity, which

we call the “Bubble Constant”, is dependent only on the mixture itself, and its values for different mixtures are given in Table 2.2.

2.4.2 Mixture Dew Point Volume Estimation

For the dew volume estimation we first tried an analogous definition to that given in Equation 2.1 for the bubble point volume. It was immediately clear such a definition did not work however, giving an unphysical behaviour. Specifically, we found that it predicted a mixture dew point volume higher than that of the pure carbon dioxide dew volume at the same temperature, which is impossible. We felt this discrepancy was due to the difference in liquid and vapour compressibilities, and it necessitated a slight deepening of our definition for dew volume estimations.

As a result, we introduced the concept of the temperature-dependent “Dew Ratio”, $\Upsilon(T)$ in order to bring the dew volume estimates back into the region of relevance. The dew ratio $\Upsilon(T)$ was defined as being the ratio of the difference in volume between the pure CO₂ dew volume and the pure N₂ volume at the same temperature, and the difference in volume between the pure CO₂ bubble volume and the pure N₂ volume at the same temperature. It is a dimensionless scaling factor which is dependent on the mixture components as well as the temperature. It must necessarily take a value between 0 and 1, and at each temperature was calculated by:

$$\Upsilon_{\text{MIX}} := \frac{v_{\text{N}_2} - w_{\text{CO}_2}}{v_{\text{N}_2} - u_{\text{CO}_2}}. \quad (2.2)$$

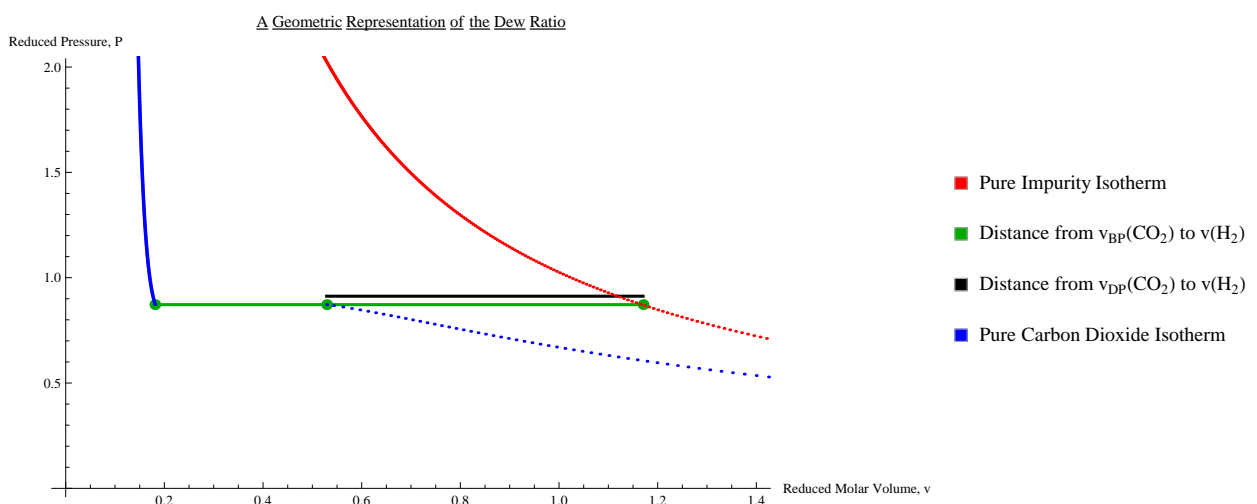


Figure 2.1: A graphical representation of the geometric quantities used in calculating the Dew Ratio, Υ

We could then give the definition for the estimated dew volume as

$$\tilde{w}_{\text{MIX}} := y_{\text{N}_2}^{\xi_{\text{DP}}} v_{\text{CO}_2} + v_{\text{N}_2} (\Upsilon_{\text{MIX}} (1 - y_{\text{N}_2}^{\xi_{\text{DP}}}) + (y_{\text{N}_2} - x_{\text{N}_2})^{\chi_{\text{DP}}}), \quad (2.3)$$

where \tilde{w}_{MIX} is the estimated bubble volume of the mixture at the required temperature and pressure, y_{N_2} is the concentration of nitrogen in the vapour phase as quoted in the literature, x_{N_2} is the coexisting mole fraction in the liquid phase, with ξ_{DP} , which we call the “Dew Constant”, and χ_{DP} , which we call the “Critical Constant” playing a similar role to the quantity ξ_{BP} introduced earlier. We note that the presence of the second term in the large bracket on the right-hand-side of Equation (2.3) ensures correct asymptotic behaviour as the pressure increases and the top of the phase boundary is reached, by ensuring that at this point,

$$\tilde{u}_{\text{MIX}} = \tilde{w}_{\text{MIX}} \quad (2.4)$$

As mentioned, the Bubble Constant ξ_{BP} , the Dew Constant ξ_{DP} , and the Critical Constant χ_{DP} are dependent only on the mixture itself, and were empirically determined by trial and error until Equations (2.1) and (2.1) gave visually good estimations. We state the values for these quantities for the binary mixtures $\text{CO}_2\text{--N}_2$, $\text{CO}_2\text{--H}_2$, and $\text{CO}_2\text{--O}_2$ which we found to allow good approximations to the VLE volumes we were seeking:

| Mixture | ξ_{BP} | ξ_{DP} | χ_{DP} |
|---------------------------|-------------------|-------------------|--------------------|
| $\text{CO}_2\text{--N}_2$ | 1.25 | 0.68 | 1.01 |
| $\text{CO}_2\text{--H}_2$ | 1.51 | 0.48 | 1.19 |
| $\text{CO}_2\text{--O}_2$ | 1.55 | 0.47 | 0.73 |

Table 2.2: A summary of the values for ξ_{BP} , ξ_{DP} , and $\bar{\xi}_{\text{DP}}$ which we used

During the fitting stages of this project, where the literature data did contain the volumes, we would use these rather than our volume estimation method, instead reserving this for the scenario where the volumes were missing. We highlight the major benefit of this method as being that it allows a substitute value for the missing coexisting volumes, which often were not quoted, to be calculated using only the pure density data which was readily available through NIST [74] and the coexisting molar fractions, which often were quoted.

2.4.3 Performance of Our Volume Estimation Method

Of course, it was necessary to ensure that the volume estimation method functioned appropriately. We did this by employing the method to estimate volumes for a se-

lection of data sets which did contain the volumes, and testing against those data sets to check the method reconstructed the volume data with reasonable accuracy. We reiterate that the volume estimation method only needed the pure density data and the coexisting mole fractions.

We carried out this test for the CO₂–N₂ system at 273.15K [54] and 288.15K [53], for the CO₂–H₂ system at 258.15K and 273.15K [92], and for the CO₂–O₂ system at 273.15K [54]. The comparisons of these estimations with the quoted data are given in Tables 2.3, 2.4, and 2.5.

| $T(K)$ | $P(\text{MPa})$ | v_{BP} % Error | v_{DP} % Error |
|--------|-----------------|------------------|------------------|
| 273.15 | 3.792 | 1.269 | 10.320 |
| 273.15 | 4.137 | 2.718 | 12.772 |
| 273.15 | 4.482 | 4.263 | 13.365 |
| 273.15 | 4.826 | 5.493 | 12.653 |
| 273.15 | 5.171 | 6.527 | 10.975 |
| 273.15 | 5.516 | 9.834 | 9.111 |
| 273.15 | 5.861 | 8.386 | 6.507 |
| 273.15 | 6.205 | 9.322 | 5.150 |
| 273.15 | 6.550 | 9.890 | 4.283 |
| 273.15 | 6.895 | 10.931 | 2.536 |
| 273.15 | 7.240 | 11.383 | 1.315 |
| 273.15 | 7.584 | 12.254 | 0.849 |
| 273.15 | 7.929 | 12.652 | 0.202 |
| 273.15 | 8.274 | 12.961 | 1.112 |
| 273.15 | 8.618 | 13.154 | 2.403 |
| 273.15 | 8.963 | 13.147 | 3.481 |
| 273.15 | 9.308 | 13.237 | 3.459 |
| 273.15 | 9.653 | 13.044 | 4.476 |
| 273.15 | 9.997 | 13.262 | 6.535 |
| 273.15 | 10.342 | 12.900 | 7.725 |
| 273.15 | 10.687 | 12.454 | 8.790 |
| 273.15 | 11.032 | 11.393 | 9.822 |
| 273.15 | 11.376 | 9.905 | 11.406 |
| 273.15 | 11.721 | 8.052 | 12.666 |
| 273.15 | 11.893 | 5.299 | 14.720 |
| 273.15 | 11.997 | 2.534 | 17.365 |
| 288.15 | 5.695 | 1.6 | 9.0 |
| 288.15 | 6.737 | 2.7 | 4.0 |
| 288.15 | 7.589 | 3.1 | 1.1 |
| 288.15 | 8.105 | 2.6 | 3.5 |
| 288.15 | 8.509 | 1.6 | 7.2 |
| 288.15 | 9.069 | 0.2 | 14.1 |
| 288.15 | 9.463 | 3.9 | 16.3 |
| 288.15 | 9.642 | 6.5 | 19.6 |
| 288.15 | 9.756 | 12.7 | 24.08 |

Table 2.3: A summary of the performance of our volume estimation method for the binary system carbon dioxide–nitrogen

| $T(K)$ | $P(\text{MPa})$ | v_{BP} % Error | v_{DP} % Error |
|--------|-----------------|------------------|------------------|
| 258.15 | 6.915 | 7.401 | 9.358 |
| 258.15 | 13.789 | 8.375 | 2.294 |
| 273.15 | 6.895 | 8.469 | 1.376 |
| 273.15 | 13.796 | 11.112 | 2.205 |

Table 2.4: A summary of the performance of our volume estimation method for the binary system carbon dioxide–hydrogen

| $T(\text{K})$ | $P(\text{MPa})$ | v_{BP} % Error | v_{DP} % Error |
|---------------|-----------------|-------------------------|-------------------------|
| 273.15 | 3.792 | 0.145 | 8.803 |
| 273.15 | 4.137 | 2.035 | 14.095 |
| 273.15 | 4.482 | 1.088 | 16.838 |
| 273.15 | 4.826 | 1.624 | 17.906 |
| 273.15 | 5.171 | 2.081 | 18.657 |
| 273.15 | 5.516 | 2.453 | 18.269 |
| 273.15 | 5.861 | 2.809 | 17.297 |
| 273.15 | 6.205 | 2.985 | 15.580 |
| 273.15 | 6.550 | 3.145 | 13.998 |
| 273.15 | 6.895 | 3.598 | 11.245 |
| 273.15 | 7.239 | 3.757 | 9.069 |
| 273.15 | 7.584 | 3.727 | 7.558 |
| 273.15 | 7.929 | 3.641 | 5.570 |
| 273.15 | 8.274 | 3.481 | 3.616 |
| 273.15 | 8.618 | 3.311 | 1.910 |
| 273.15 | 8.963 | 3.050 | 0.095 |
| 273.15 | 9.308 | 2.739 | 2.264 |
| 273.15 | 9.653 | 2.417 | 4.474 |
| 273.15 | 9.997 | 2.314 | 7.390 |
| 273.15 | 10.342 | 1.562 | 9.796 |
| 273.15 | 10.687 | 0.744 | 11.998 |
| 273.15 | 11.032 | 0.426 | 13.320 |
| 273.15 | 11.376 | 2.846 | 11.965 |
| 273.15 | 11.549 | 4.107 | 10.886 |
| 273.15 | 11.742 | 16.043 | 2.124 |

Table 2.5: A summary of the performance of our volume estimation method for the binary system carbon dioxide–oxygen

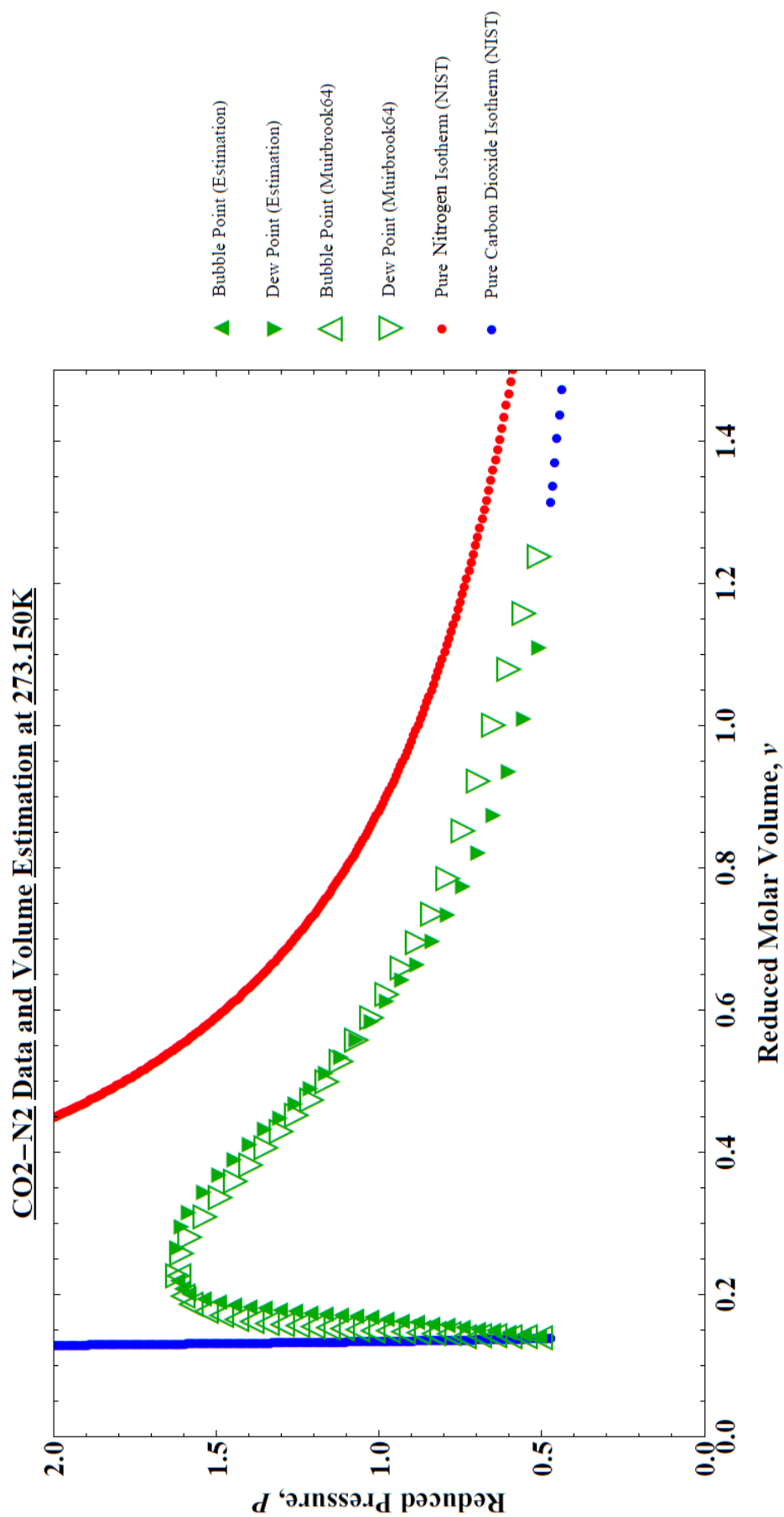


Figure 2.2: Behaviour of the volume estimation method compared to literature data at 273.15K for a carbon dioxide–nitrogen mixture

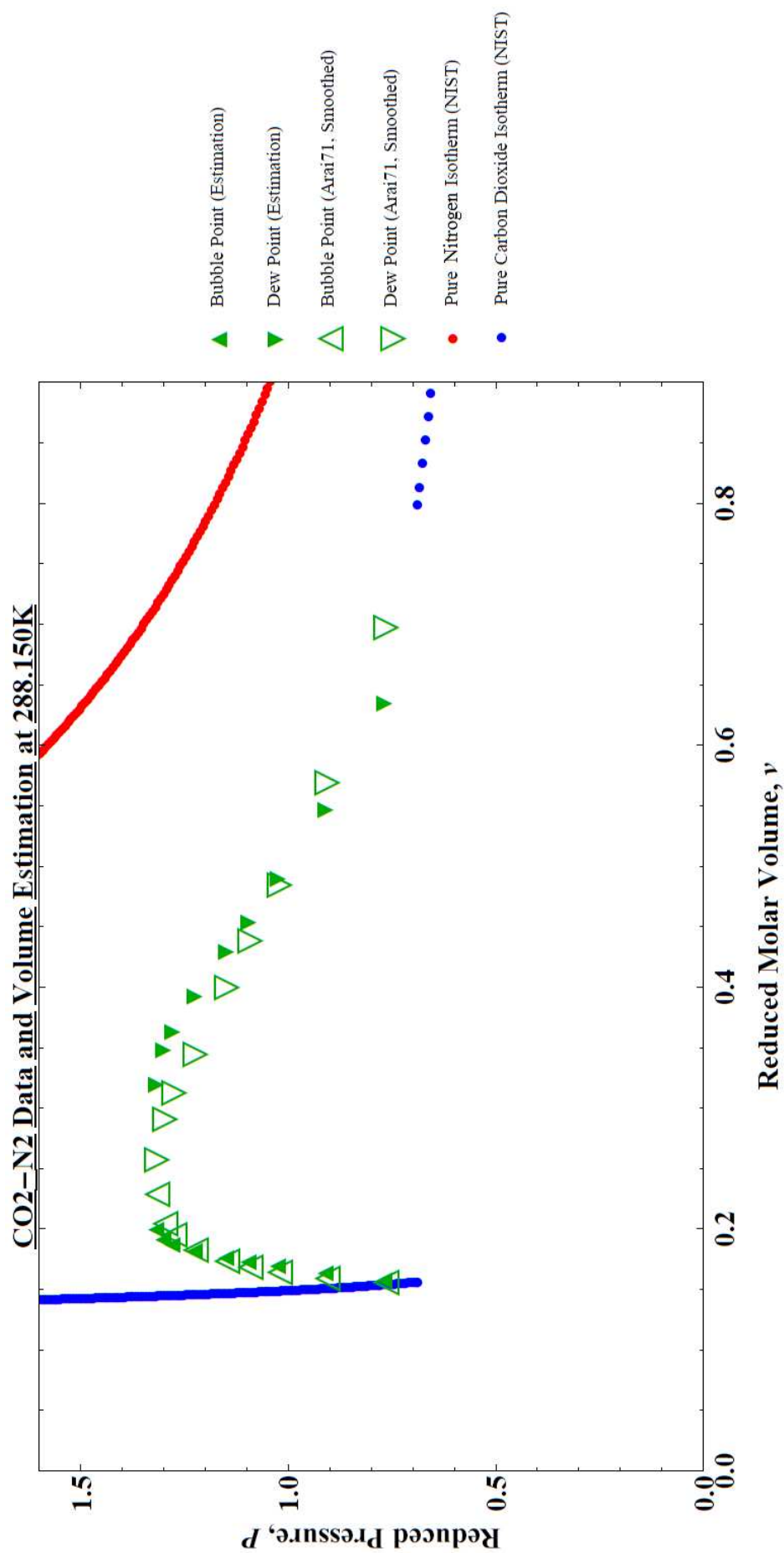


Figure 2.3: Behaviour of the volume estimation method compared to literature data at 288.15K for a carbon dioxide–nitrogen mixture

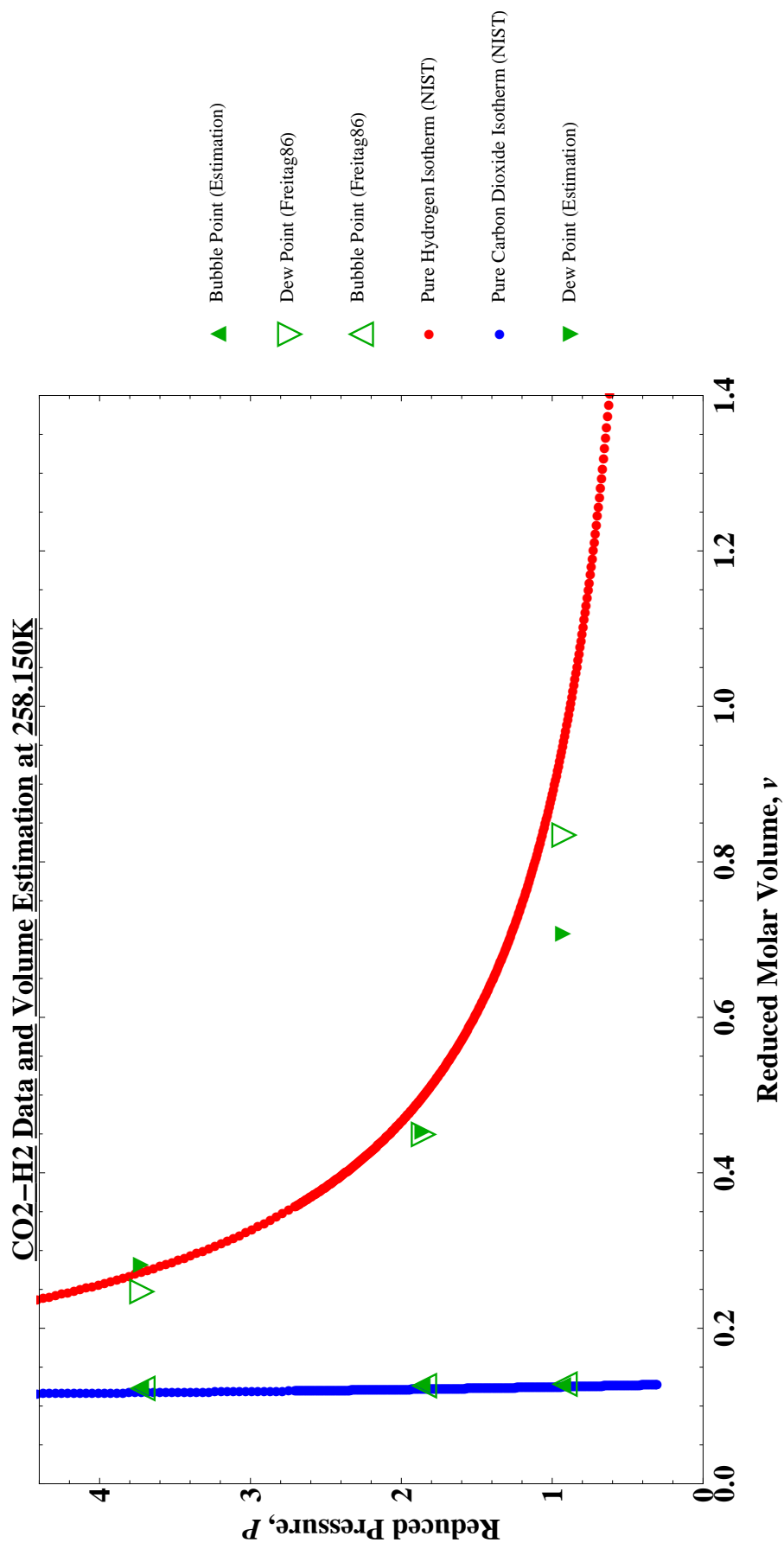


Figure 2.4: Behaviour of the volume estimation method compared to literature data at 258.15K for a carbon dioxide-hydrogen mixture

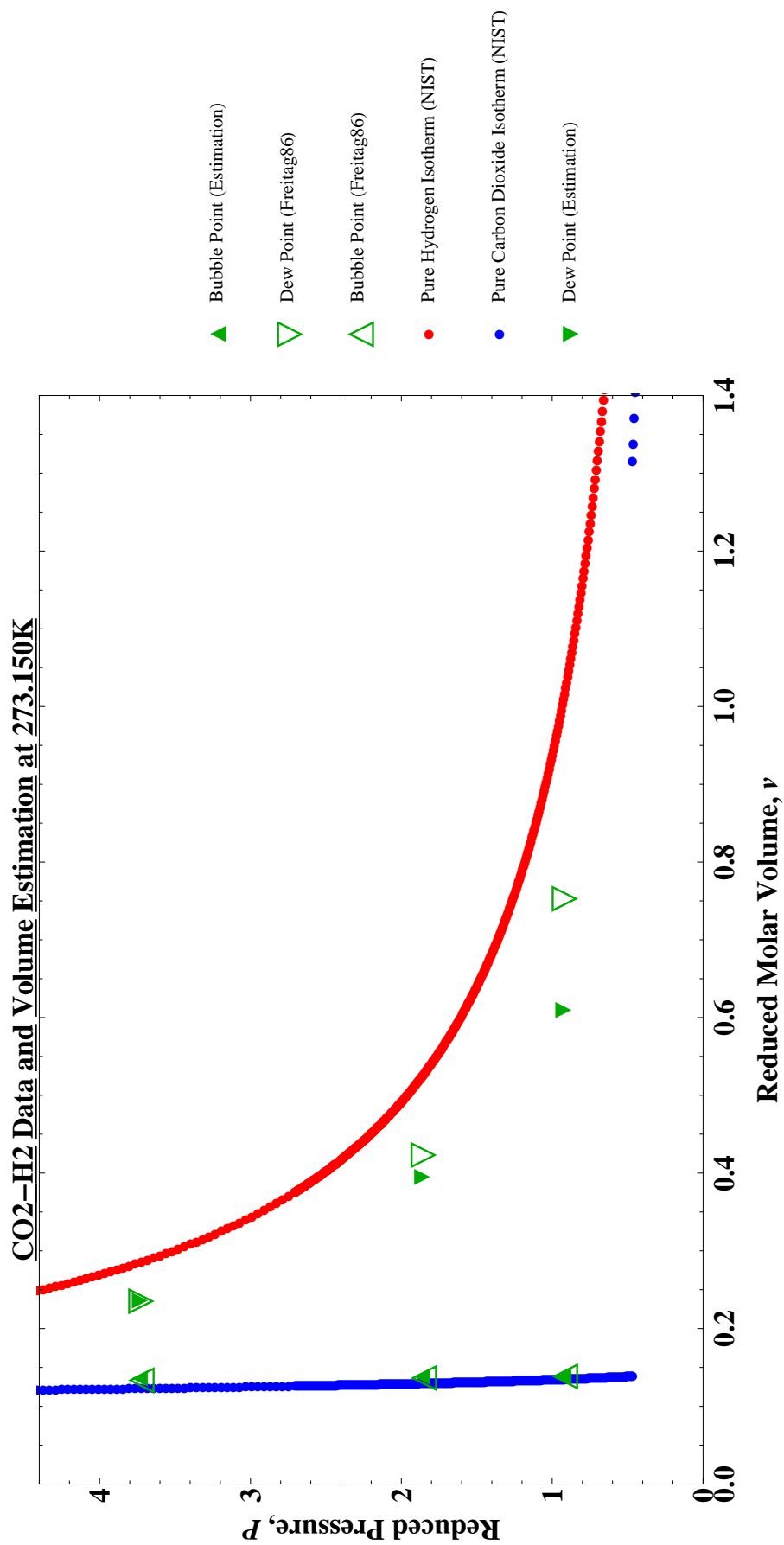


Figure 2.5: Behaviour of the volume estimation method compared to literature data at 273.15K for a carbon dioxide-hydrogen mixture

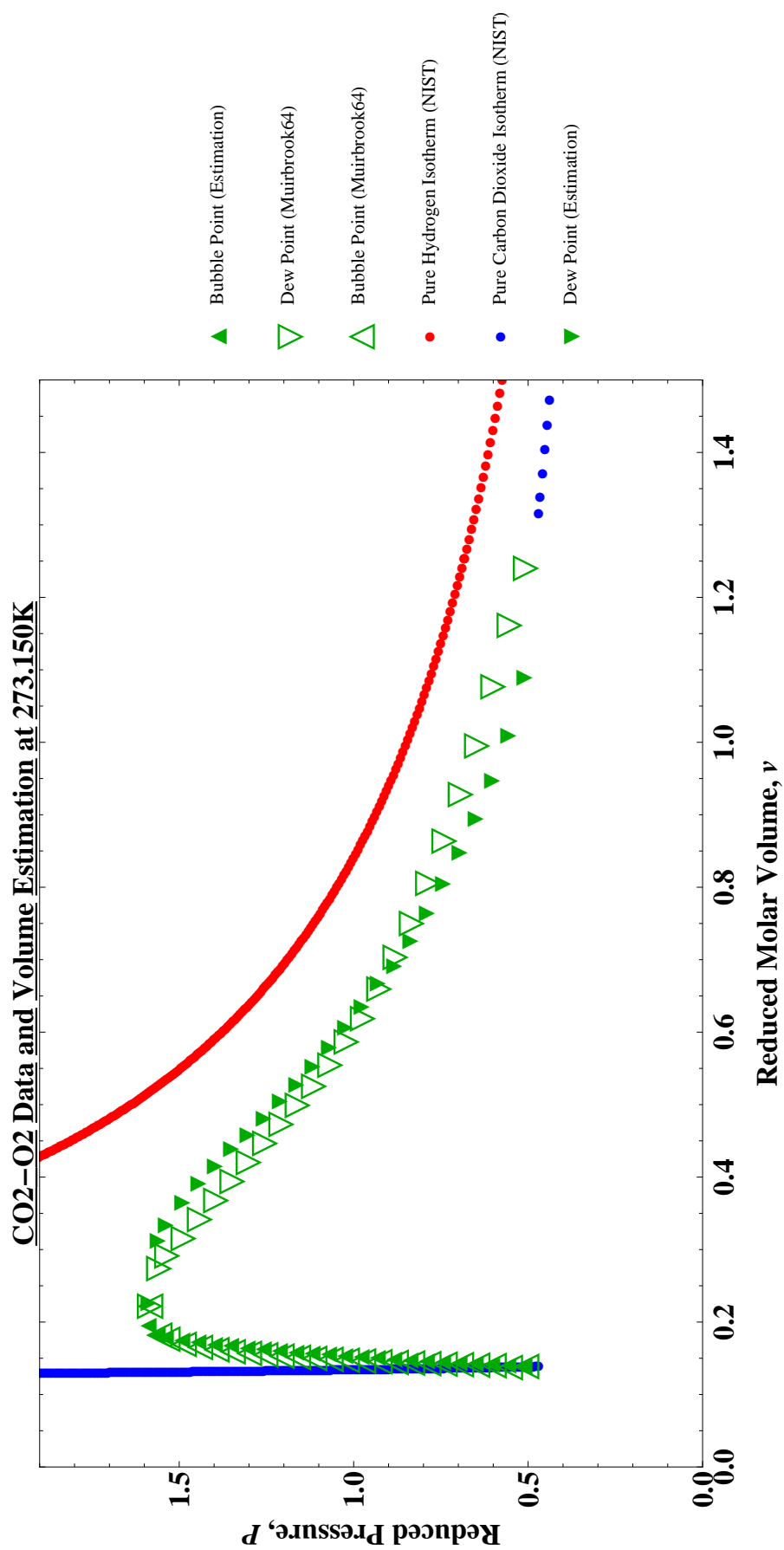


Figure 2.6: Behaviour of the volume estimation method compared to literature data at 273.15K for a carbon dioxide–oxygen mixture

In the binary system $\text{CO}_2\text{--N}_2$ our estimation method recovered the volumes with an average percentage error of 7.95% and a maximum percentage error of 24.08%, for $\text{CO}_2\text{--H}_2$ with an average percentage error of 6.32% and a maximum percentage error of 11.11%, whilst in the binary system $\text{CO}_2\text{--O}_2$ it recovered them with an average percentage error of 3.05% and a maximum percentage error of 18.66%. We felt that these accuracy figures were very similar to the anticipated level of accuracy of the majority of experimental thermodynamic measurements of the type reported in the literature, so on this basis, felt confident that we could employ our volume estimation method to reconstruct the missing data from the literature with a similar accuracy to that with which it would have been presented anyway.

We acknowledge the limitation of this method that it only appeared to give valid estimations within the temperature range from around 260K to 300K: In attempting to estimate the carbon dioxide–nitrogen data at 303.3K, we found the method to perform badly enough that we could not use the resultant estimations. We also note that in the system containing hydrogen, at 258.15K, in Figure 2.4, the estimation of the dew point at the highest pressure was also invalid, and we neglected this estimation for subsequent fittings. Nevertheless, we generally considered that this method would be extremely valuable in substituting for the missing coexisting volumes.

2.5 Estimation of Homogeneous Phase Molar Volumes

Since we were trying to fit to two types of data, and bearing in mind that there were very few temperatures where both VLE and homogeneous density data existed, we felt it would be beneficial for the fitting regimes to extend the volume estimation method described in Section 2.4 to also include estimations for mixture molar volumes in the homogeneous liquid and vapour phases. This was necessary as we wished to constrain the model to give physically relevant homogeneous density predictions, even in situations where this data was not available.

2.5.1 Liquid Phase Volume Estimation

For the liquid phase molar volume estimations we again did this by a weighted average between the pure carbon dioxide molar volume and that of the second component in the binary mixture, where the weighting constant was defined so as

to give consistent behaviour approaching the liquid saturation line:

$$\lambda = \frac{\tilde{u}_{\text{MIX}} - v_{\text{CO}_2}}{v_{\text{N}_2} - v_{\text{CO}_2}}, \quad (2.5)$$

where for any given temperature and pressure, \tilde{u}_{MIX} is the coexisting bubble volume estimated by the method in Section 2.4, and v_{CO_2} and v_{H_2} are the pure molar volumes for carbon dioxide and nitrogen (or respectively, whichever the second component in the mixture is) at the given temperature and pressure. We then defined the liquid phase mixture volume to be

$$\tilde{v}_{\text{MIX}} = (1 - \lambda)v_{\text{CO}_2} + \lambda v_{\text{N}_2}. \quad (2.6)$$

We found it useful to establish the homogeneous phase volumes up to the limit of the phase boundary. We reiterate that that quantity λ ensures behaviour is consistent upto the phase boundary, as shown in Figure 2.7

2.5.2 Vapour Phase Volume Estimation

The vapour phase volume estimation was a little more straightforward as the weighting constant was simply taken to be the molar concentration of the impurity:

$$\tilde{v}_{\text{MIX}} = (1 - y_{\text{N}_2})v_{\text{CO}_2} + y_{\text{N}_2}v_{\text{N}_2}, \quad (2.7)$$

where y_{N_2} is the concentration of impurity in the vapour phase. We note that since at the transition from vapour phase through the multi-phase region and into the liquid phase the molar volume of the pure carbon dioxide jumps suddenly, this definition was only valid upto the vapour pressure at the given temperature, and that these volume estimations for the vapour phase could not therefore be extended all the way to the two-phase boundary.

2.5.3 Behaviour of the Homogeneous Phase Volume Estimation

There was no homogeneous volume data to compare this method to so we are unable to specify its performance in terms of a percentage error. We can however illustrate that it gave a physically relevant behaviour in both the liquid and vapour phases as shown in Figures 2.7 and 2.8.

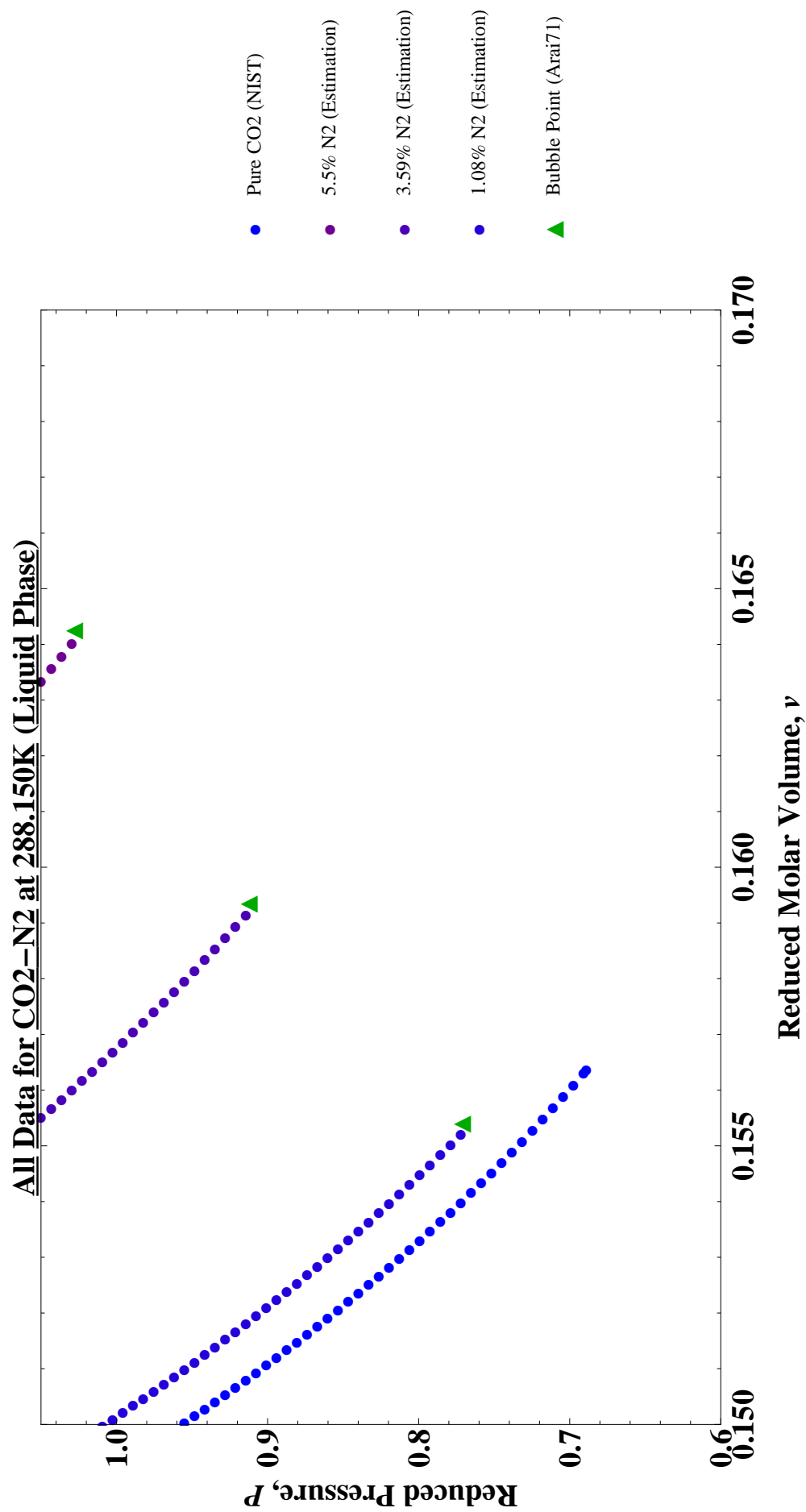


Figure 2.7: Behaviour of the volume estimation method in the liquid phase, upto the bubble point, at 288.15K for a carbon dioxide–nitrogen mixture

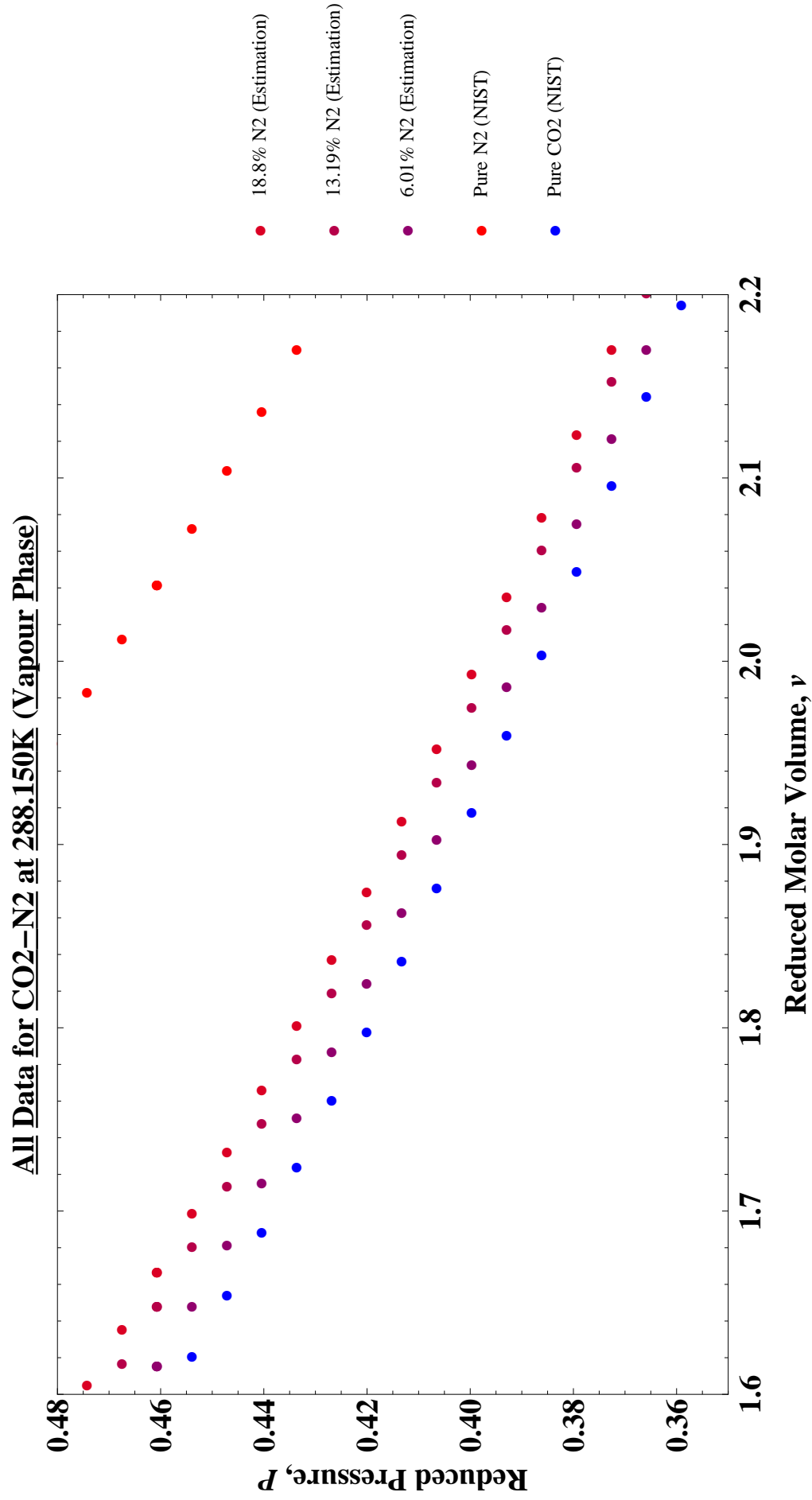


Figure 2.8: Behaviour of the volume estimation method in the vapour phase at 288.15K for a carbon dioxide–nitrogen mixture

2.5.4 Benefits of the Homogeneous Phase Volume Estimation

We felt the benefits of the homogeneous phase mixture volume estimation method were clear as, supplemented with the VLE coexisting volume method outlined in Section 2.4, it allowed us to construct a framework of data against which to fit the proposed equation of state. Without these methods, we would simply have been unable to do this in a meaningful way. The true value of these two methods combined, given that we had identified very few temperatures where homogeneous density and VLE data were both given, was that it meant we could fit the model at any temperature at which merely VLE data was given, and that even then, it needn't have contained the molar volumes.

In terms of attempting to fit the model to as many data points as possible in order to incorporate as much physical relevance to the model as possible, we considered this to be highly beneficial.

2.6 Mathematical Techniques Used for Fitting

At this point we highlight that we viewed our method as one of mathematical modelling, as opposed to physical modelling. Our outlook was that the parameters of the system were quantitative tools that allowed us to fit the proposed model to the data, and any dimensional equivalence with physical quantities is purely coincidental. We list here the main mathematical techniques used for fitting the model to the data which we used in our work.

2.6.1 Simulated Annealing

Simulated annealing [93, 94] is a process of global non-linear optimisation, a technique we used to start our method of fitting to the literature data. It is a stochastic process which searches extensively throughout a parameter space to find an optimum solution, working particularly well in scenarios where a desired global optimum may be hidden amongst a large number of mere local optima.

The term “annealing” stems from the analogy of this process to the cooling of liquids into crystalline structures, in which a slow cooling will permit large crystals of a low energy state to be formed, whereas fast cooling will limit the size of the crystals to be formed, whereby a higher energy state will have been achieved. The key is that by cooling slowly, the individual atoms can mobilise into positions al-

lowing the larger crystal to be formed, but under a quick cooling, energy is lost too quickly and the atoms cannot align to form such large structures in time.

The important feature of simulated annealing is that, just as slowly cooling atoms can retain enough kinetic energy despite the diminishing thermal energy in order to move into an optimal position, it can search through a parameter space in such a way that it may occasionally move against a gradient. This prevents a scenario whereby it doesn't automatically find the nearest local optima, but can have a chance to find the desired global optimum, or at least a very good local optimum. Traditional downhill methods of optimisation do not allow for this as their algorithmic greediness will not allow the search to progress away from the nearest optimum, and in doing so, will very rarely yield the global optimum.

This means that simulated annealing is perfect for our requirement of finding a desired optimum in a large and potentially complicated parameter space containing a multitude of local optima, as it will not get stuck in the wrong location. Specifically, it works best in scenarios where there may be very many (perhaps arbitrarily many) local optima, in which case traditional downhill search algorithms cannot (usually) hope to find the global optimum. It searches by looking over wide areas to begin with before determining where the best local optima are likely to be located, and zooming in on these areas, repeating this process until a “good” local optimum which may approximate the global optimum is found. In this way, simulated annealing cannot be assumed to always give the very best possible solution, but it will usually return an optimum that gives very good approximations to it. Given that we are going to be searching high-dimensional parameter spaces whilst using our method, an exact optimum is not always necessary for our application; just a good approximation of it. To this end, simulated annealing is a method which is easily accessible in Wolfram Mathematica under the “NMinimize” command. It is a sufficiently powerful tool for us to not need to worry about the results it will return to us, as we deemed it suitable to use in order to produce an initial set of parameters to fit to data where no previous solutions had been determined. We were able to tailor our use of simulated annealing by altering the various search parameters offered by Mathematica: “SearchPoints” allowed us to control with how many simultaneous attempts the algorithm would search the landscape for an optima, “PerturbationScale” would control the size of the jumps the routine took in searching the landscape, and “MaxIterations” controlled how long the routine would look for before declaring itself to have found or not found an optimum.

2.6.2 Local Minimisation

Local minimisation is fundamentally different to simulated annealing in so far as it cannot under any circumstances usually hope to find a global optimum. It finds a local optimum in a perfunctory way by employing a standard downhill simplex method [94] to find a location in the parameter space at which a local optimum occurs, even though it may not be close in value to the true global optimum. This is the main difference to simulated annealing.

In addition, where simulated annealing does not need to have a starting location for its search specified, local minimisation does, and goes “downhill” from there. For application in our method this was actually beneficial as we could use the optimal solution from the previous temperature point as the starting point for the search for parameter values at the new temperature, and in doing so, hope to ensure smoothness of the temperature-dependent variation of each parameter. Another key difference between simulated annealing and local minimisation was the deterministic nature of local minimisation, used in Mathematica under the command “FindMinimum”. This means that given a particular starting point local minimisation will always find its way to the same optimum, as it employs a gradient-based method to search for any local minimum. The major drawback of this is that sometimes we found the “FindMinimum” command converging to optima that were irrelevant to us, in which case we had to manipulate other search parameters to persuade it to find one which was acceptable. One benefit of local minimisation over simulated annealing was that it tended to converge quicker, due to the deterministic nature, resulting in reduced uncertainty, in its direction of search. Local minimisation was also controlled in Mathematica by a set of search parameters: “AccuracyGoal” would control how close to the actual optimum we wanted the routine to get, “PrecisionGoal” would control the number of significant figures quoted in the output, “WorkingPrecision” would control the extent to which inter-stage rounding errors could build up to affect the final answer, and “MaxIterations” was as with simulated annealing. We used local minimisation in our work to find parameter values after the initial set had been found using simulated annealing.

2.7 Creating the Fugacity Constraints

2.7.1 The Fugacity of A Chemical Component when in Mixture

Equation (1.19) gives us the fugacity of a single particular chemical component whilst in mixture. Setting $V = Nv$, where V is the total volume, v is the molar volume, and N is the number of moles of the substance, we get

$$\log_i(\bar{\phi}(v)) = \frac{1}{RT} \int_{\hat{v}=\infty}^{\hat{v}=v} \left(\frac{RT}{\hat{v}} - \left(\frac{\partial P}{\partial N_i}(\hat{v}) \right)_{T, \hat{v}, N_{j \neq i}} \right) d\hat{v} - \log \left(\frac{RT}{Pv} \right), \quad (2.8)$$

where the bar in “ $\bar{\phi}$ ” denotes that this is the mixture fugacity as opposed to pure case fugacity, and the subscript i denotes the chemical species being referred to in this equation. After the following non-dimensionalisation to allow all variables to take similar numerical values:

$$P = P_c P^*, \quad (2.9)$$

$$T = T_c T^*, \quad (2.10)$$

$$v = \left(\frac{RT_c}{P_c} \right) v^*, \quad (2.11)$$

this becomes:

$$\log_i(\bar{\phi}) = \frac{1}{T} \int_{\hat{v}=\infty}^{\hat{v}=v} \left(\frac{T}{\hat{v}} - \left(\frac{\partial P}{\partial N_i}(\hat{v}) \right)_{T, \hat{v}, N_{j \neq i}} \right) d\hat{v} - \log \left(\frac{Pv}{T} \right), \quad (2.12)$$

with all quantities in this expression being the non-dimensional equivalents. Equation (2.12) will have to be used repeatedly in our work in ensuring correct mixture VLE predictions. In order to achieve a state of thermodynamic equilibrium between different chemical components and different phases within those components, we require that the volumes given by each of these are matched at the point of equilibrium.

2.7.2 Pure Substance Fugacity

Equation (1.18) gives us the fugacity of a pure substance. Again setting $V = Nv$, we get

$$\log(\phi(v)) = \frac{1}{RT} \int_{\hat{v}=\infty}^{\hat{v}=v} \left(\frac{RT}{\hat{v}} - P(\hat{v}) \right) d\hat{v} - \log \left(\frac{Pv}{RT} \right) + \left(\frac{Pv}{RT} \right) - 1 \quad (2.13)$$

and after the same nondimensionalisation as in Equations (2.9) — (2.11) this becomes:

$$\log(\phi) = \frac{1}{T} \int_{\hat{v}=\infty}^{\hat{v}=v} \left(\frac{T}{\hat{v}} - \frac{\partial P}{\partial N}(\hat{v}) \right) d\hat{v} - \log\left(\frac{Pv}{T}\right) + \left(\frac{Pv}{T}\right) - 1, \quad (2.14)$$

again with all quantities in this expression being the non-dimensional equivalents. Equation (2.14) will also have to be used repeatedly in this work in ensuring correct pure VLE predictions.

Chapter 3

Formulation of the Model

3.1 Physical Constraints and Expected Qualitative Behaviour of an Equation of State

As established in the opening chapter, we aimed to propose a new equation of state which was simultaneously both sufficiently accurate and easy to implement. We aimed for the simplicity element to be achieved by our proposal of a model with an appropriate degree of functional complexity. In particular, we set out to only permit an EoS containing rational functions. To ensure relevance and accuracy of behaviour, there were two sets of physical constraints that the model had to satisfy. Firstly, we required that an accurate description of the volume–pressure relation must always be given. Next, for the pure case, at the critical temperature T_c the critical pressure P_c must be predicted at the critical molar volume v_c . This gave us the constraint:

$$P(v_c, T_c) = P_c, \quad (3.1)$$

where T_c , P_c , and v_c were as quoted in Table 1.4 for CO_2 . At this temperature, there must also be a saddle point in $P(v)$ at the critical molar volume, yielding two more constraints:

$$\frac{\partial^2 P}{\partial v^2}(v_c, T_c) = \frac{\partial P}{\partial v}(v_c, T_c) = 0. \quad (3.2)$$

Recalling the aim for the equation to be able to model the phase behaviour accurately, it was necessary that, at sub-critical temperatures, we could accurately

predict the bubble point ($v_{\text{BP}}, P_{\text{vap}}$) and the dew point ($v_{\text{DP}}, P_{\text{BP}}$), where v_{BP} is the molar volume at which the bubble point occurs, v_{DP} is the molar volume at which the dew point occurs, and P_{vap} is the vapour pressure corresponding to both. In order to do this, we observed that at the bubble and dew volumes the fugacity for each chemical component (see Section 2.7 on VLE and fugacity) should be matched and therefore that Equation (1.18) evaluated at these two volumes should take equal values. In addition, the model must ensure that the predicted pressure at each of the the bubble and dew volumes was equal to the vapour pressure. Thus, for temperatures below T_c , we had two sets of constraints to impose; those ensuring correct pressures at the points of coexistence were described:

$$P(v_{\text{BP}}) = P_{\text{vap}}, \quad (3.3)$$

$$P(v_{\text{DP}}) = P_{\text{vap}}, \quad (3.4)$$

and those ensuring correct phase behaviour are described:

$$\log \phi(v_{\text{BP}}) = \log \phi(v_{\text{DP}}). \quad (3.5)$$

In Equations (3.3) to (3.5), v_{DP} , v_{BP} , and P_{vap} were values given by NIST. We use Equation (1.18) to enforce the constraint in Equation (3.5).

At super-critical temperatures there were no phase behaviour constraints as there could be no VLE there, and we were free to focus entirely on fitting to the density experimental data. These physical constraints were incorporated into fitting of the proposed model at the critical temperature by imposing Equations (3.1) and (3.2) and below the critical temperature by imposing Equations (3.3) to (3.5).

For the case of binary mixtures we again had two types of constraint to impose in order to ensure correct physical behaviour. Once more we had to impose the condition that correct pressures were predicted at the mixture bubble and dew points:

$$P(v_{\text{BP,MIX}}) = P_{\text{vap,MIX}}, \quad (3.6)$$

$$P(v_{\text{DP,MIX}}) = P_{\text{vap,MIX}}, \quad (3.7)$$

as well as to ensure that the fugacity at each of these coexisting volumes for each different chemical species within the mixture was the same

$$\log \bar{\phi}_i(v_{\text{BP}}) = \log \bar{\phi}_i(v_{\text{DP}}), \quad (3.8)$$

where $P(v)$ is the formulation we propose, $v_{\text{BP},\text{MIX}}$ is the molar volume at the bubble point, $v_{\text{DP},\text{MIX}}$ is the molar volume at the dew point, $P_{\text{vap},\text{MIX}}$ is the vapour pressure of the mixture at these volumes, and $\bar{\phi}_i$ denotes the mixture fugacity for component i as opposed to ϕ_i which denotes the fugacity of pure component i . Thus, there would be as many constraints of the type shown in Equation (3.8) as there were components in the mixture.

3.2 Finding Vapour–Liquid Equilibrium

In the pure case, we are able to compute VLE by solving for the three unknown variables v_{BP} , v_{DP} and P_{DP} from the three Equations (3.3) to (3.5) for each temperature step. This required parameter values at the given temperature to be known so that $P(v)$ would be fully determined. We thus highlight the distinction between the initial process of finding parameter values which allowed the model to fit the data, and the subsequent process of implementing these parameter values and solving the system of three unknowns in three equations to generate a picture of the VLE behaviour of the system.

For binary mixtures this situation is the same, but there are four variables v_{BP} , v_{DP} , the composition of the liquid phase x_{CO_2} and the composition of the vapour phase y_{CO_2} from the four equations, noting that in a binary case Equation (3.8) yields two constraints; one each for both components. Again, we highlight that before this stage can be carried out, fitting to the data to find parameter values that would allow $P(v)$ to be defined would have had to have been done beforehand. In solving this system of equations we can thus find the binary mixture VLE for any specified temperature and the pressure.

This would allow us to calculate the VLE. Whether fitting the model to the data in the pure case or in a binary mixture however, it was also as necessary to ensure that correct pressure behaviour was described by the model. In the case of modelling the pure CO_2 we took the pressure data from the NIST database and included this data in the fitting regime to ensure the model could give accurate pressure descriptions. Whilst modelling mixtures, we again took both of the pure case pressure data sets from NIST, and any available pressure data for intermediate mixtures found within the literature, a comprehensive review of which was included in the Appendices.

3.3 Proposed Equation of State

We began the quest for a new functional form of equation that would satisfy the aims set out in Chapter 1 by considering the advantages and disadvantages of the most commonly used Equations [36]. We then used the general form of the many existing cubic equations of state as a template. As most of these equations were all modifications to the van der Waals equation, itself an adaptation of the ideal gas law, this was the starting point for our search. We decided early on that a pressure explicit equation of the form $P(v, T)$, would allow us both to calibrate against the data and to incorporate the fugacity constraints discussed previously most easily.

The evolution in functional forms from the ideal gas law towards the PREoS and beyond to the SWEoS, as noted in the literature review was used as a motivation for the type and complexity of the function we should be looking for in terms of both the degree and the number of parameters within. The equation we chose, having tried many variations on this theme, and the equation of state we propose as part of this thesis is:

$$P(v, T; a, b, c, d, e, f, g) = \frac{RT}{v + a} - \frac{b^2}{v^2 + c^2} - \frac{d^3}{v^3 + e^3} + \left(\frac{f}{v - g} \right)^6 \quad (3.9)$$

Immediately we are able to verify that this equation satisfied the requirement of being functionally quite easy to manage, there are relatively few terms (only four) and relatively few parameters (only seven), which most modern computers and software should have little problem in manipulating and using to perform calculations. From here it was a matter of also satisfying the primary requirement of giving accurate pressure and phase behaviour predictions compared with the compiled data. To do this we proceeded by determining the combination of the seven parameter values which best allowed Equation (3.9) to describe the data. This was done by the process of finding an initial set of parameter values using simulated annealing then subsequent values at different temperatures using local minimisation, as mentioned in the methodology in Chapter 2.

In Equation (3.9), P was the pressure in MPa, v was the molar volume in $\text{m}^3 \cdot \text{mol}^{-1}$, T was absolute temperature in K, and a through g were parameters of the system which allowed us to fit to the data at every temperature. Our motivations for suggesting this form of equation were as follows:

- All terms ensure it exhibited behaviour resembling the ideal gas law at low pressures, with $T \rightarrow 0$ as $v \rightarrow \infty$.

- A high-powered term to allow the model to retain enough flexibility to model the liquid-like incompressibility at high pressures, including the very sharp upturn of pressure immediately above the critical point. With this in mind, the final term of (3.9) was specifically chosen with a higher power than is usually seen in equations of state of similar complexity in order to allow fitting to the steep up-turn in pressure that exists above the critical point; a feature which cubic equations of state such as PREoS frequently miss out on (see Figures 4.26 to 4.28 for an illustration).
- A suitable number of parameters to allow the model to accurately fit the elongated plateau in $P(v)$ in the region of v_c at the critical temperature.

3.4 Nondimensionalisation

Equation (3.9) was nondimensionalised according to a similar regime as used to nondimensionalise the fugacity constraints (1.18) and (1.19), by the following set of substitutions:

$$P = P_c P^*; \quad (3.10)$$

$$T = T_c T^*; \quad (3.11)$$

$$v = \left(\frac{RT_c}{P_c} \right) v^*; \quad (3.12)$$

$$a = \left(\frac{RT_c}{P_c} \right) a^*; \quad (3.13)$$

$$b = \left(\frac{(RT_c)^2}{P_c} \right) b^*; \quad (3.14)$$

$$c = \left(\frac{RT_c}{P_c} \right)^2 c^*; \quad (3.15)$$

$$d = \left(\frac{(RT_c)^3}{P_c^2} \right) d^*; \quad (3.16)$$

$$e = \left(\frac{RT_c}{P_c} \right)^3 e^*; \quad (3.17)$$

$$f = \left(\frac{RT_c}{P_c^{5/6}} \right) f^*; \quad (3.18)$$

$$g = \left(\frac{RT_c}{P_c} \right) g^*, \quad (3.19)$$

where \star denotes a dimensionless quantity. We nondimensionalised each quantity within our model against a suitable typical quantity, according to the regime noted

in Equations (3.10) to (3.19). For example, temperature T was scaled against the carbon dioxide critical temperature T_c so as to allow us to work with values which were all roughly of order 1. Crucially, we saw that this would give the numerical optimisation algorithms (simulated annealing and local minimisation) a better chance of finding good optima during the fitting process as they could focus on a particular region of the parameter space. After nondimensionalisation we had:

$$P(v^*, T^*; a^*, b^*, c^*, d^*, e^*, f^*, g^*) = \frac{T^*}{v^* + a^*} - \frac{b^{*2}}{v^{*2} + c^{*2}} - \frac{d^{*3}}{v^{*3} + e^{*3}} + \left(\frac{f^*}{v^* - g^*} \right)^6, \quad (3.20)$$

and from this point forwards we dealt exclusively with nondimensionalised units (unless otherwise stated), and dropped the \star 's for notational convenience. This yielded the dimensionless version of our equation of state:

$$P(v, T; a, b, c, d, e, f, g) = \frac{T}{v + a} - \frac{b^2}{v^2 + c^2} - \frac{d^3}{v^3 + e^3} + \left(\frac{f}{v - g} \right)^6. \quad (3.21)$$

For example, applying the proposed model (3.21) to the pure fugacity constraint defined in Equation (2.14) gave:

$$\begin{aligned} \log \phi(v) = & -\frac{f^6}{5T(g-v)^5} + \log \left(\frac{v}{a+v} \right) + \frac{d}{3Te^{2/3}} \log \left(\frac{\sqrt[3]{e} + v}{\sqrt{e^{2/3} - \sqrt[3]{e}v} + v^2} \right) \\ & + \frac{b}{T\sqrt{c}} \arctan \left(\frac{v}{\sqrt{c}} \right) + \frac{d}{T\sqrt{3e^2}} \arctan \left(\frac{2v - \sqrt[3]{e}}{\sqrt{3}\sqrt[3]{e}} \right) \\ & - \frac{\pi}{2T} \left(\frac{b}{\sqrt{c}} + \frac{d}{\sqrt{3e^{2/3}}} \right) - \log \left(\frac{P(v)v}{T} \right) + \left(\frac{P(v)v}{T} \right) - 1 \end{aligned} \quad (3.22)$$

This expression plays a key role in enforcing the coexistence constraints and finding suitable parameter values to optimise the model against the data.

Chapter 4

Calibration of the Pure Carbon Dioxide Equation

4.1 Getting the Search Started: Fitting the Critical Point

Work carried out in this chapter was presented in a published paper [40] in May 2013. For the calibration of the pure CO₂ equation we needed only data from NIST. Whereas this data was itself generated using the an equation of state, it was done so using a far more complicated version (SWEoS) [74], which has scope to be highly accurate at the cost of functional simplicity, as has already been noted. We determined that the data was thus akin to high-accuracy experimental measurements, and could be treated as such. It is worth noting that the NIST data is well known for being used as a benchmark for high accuracy, so for our purposes, we were satisfied that using it to calibrate our equation should cause no problems.

To begin with we ran the simulated annealing package discussed in the opening chapter to seek the parameter values a through g at the critical temperature T_c . This process searched the the seven-dimensional space for a good combination of these parameters which would allow the proposed dimensionless Equation (3.21) to match most closely the NIST data at this temperature. We recognised the possibility that either there was no exact match given the functional form we had proposed, in which case no combination of parameter values would suggest to us we had a perfect agreement, or that it might be the case that even if there was one, the search

algorithm might not find it.

4.1.1 Error Function

To allow us to carry out this search, we defined an error function $E(a, b, c, d, e, f, g)$, depending on the system parameters, for Equation (3.21). This would work by assigning a comparatively high score for a bad fit of the data, a lower score for a better fit of the data, and a score of zero for a perfect match. The error function was to be dependent on the parameters in such a way that by minimising the value of this error function using simulated annealing, we would find the parameter values that had brought about such an optimum. At the critical temperature, the simulated annealing search algorithm progressed through the seven-dimensional space trying out different combinations of parameters, giving us output values for parameters a to g . Again, it was important to understand that these values might not have been found at a global optimum, but merely at a good local optimum, which for our purposes was sufficient.

The error function we used was arbitrarily defined, but as long as it exhibited the property that a closer agreement to the data resulted in a lower score, it was suitable for our needs. The error function $E(a, b, c, d, e, f, g)$ which we chose to use at each temperature T was:

$$E(a, b, c, d, e, f, g) = W \left(\sum_{i=1}^n \left(\frac{P(v_{\text{NIST}}^{(i)}, T) - P_{\text{NIST}}^{(i)}}{P_{\text{NIST}}^{(i)}} \right)^2 \right) + (1 - W)\Gamma, \quad (4.1)$$

where Γ represents the type of behaviour being modelled (density and VLE in the co-existence region, just density in the homogeneous region, or the limiting behaviour between). The first term on the right-hand-side of Equation (4.1) was responsible for enforcing the density constraints whilst the second term was responsible for enforcing any coexistence constraints. We can visually verify that Equation (4.1) satisfies the requirements for the error function as outlined above. The data we took from NIST went from 0.05MPa to 20MPa, approximately three times the critical pressure for pure carbon dioxide, at intervals of 0.05MPa. We chose this range to ensure the model was fit to the CCS pipeline relevant range of pressures, but in doing so, noted that much of the literature suggested a pressure of 20MPa would be far too high for this purpose. Nevertheless, by fitting at higher pressures, we would incorporate this enhanced range of operation of the model in case it might be needed for modelling during the repressurisation stages of CCS pipelines. In this model, T_c was the critical temperature for CO_2 , taken to be the value given in Table

1.4, and the quantity $W \in [0, 1]$ was a weighting function, which we chose manually, whose role was two-fold: Firstly, it would ensure that a suitable balance between predictions of the model for VLE and pressure was found. Secondly, it would allow us to perturb the parameter values in order that we might try to impose smooth temperature dependence for each.

In Equation (4.1), the first term ensured the pressure constraints were fit, whilst the second term ensured the coexistence constraints were fit. To be consistent with our work leading up to this point, each of the quantities in Equation (4.1) were in reduced (nondimensionalised) units, again because it allowed the search algorithm to focus more closely in a particular region of the seven-dimensional parameter space rather than having to search a wider region.

Γ was a quantity which depended on the temperature at which we were fitting and had the role of capturing the coexistence behaviour. We note that whereas coexistence could only ever occur below the critical temperature, the pressure data had to be accurately modelled at every temperature point. Below the critical temperature there were the VLE coexistence constraints to be enforced, whilst at the critical temperature there were the critical point constraints, and above the critical temperature there were no extra constraints. Thus, following on from Equations (3.1) and (3.2) for fitting at the critical temperature, we set:

$$\Gamma = \left(P(v, T) \Big|_{v=v_c, T=T_c} - P_c \right)^2 + \left(\frac{dP}{dv}(v, T) \Big|_{v=v_c, T=T_c} \right)^2 + \left(\frac{d^2P}{dv^2}(v, T) \Big|_{v=v_c, T=T_c} \right)^2, \quad (4.2)$$

and this fully defined our error function $E(a, b, c, d, e, f, g)$ which we could then ask simulated annealing to work with, because our equation of state was dependent on temperature, molar volume, and each of the parameters $P(v, T; a, b, c, d, e, f, g)$. We note at this point that all the quantities in the error function E were squared quantities, thus imposing the restriction that E could never take a negative value, and only take a zero value if the NIST data were fully satisfied was ensured. This fulfilled our requirement for it to act as an error function.

The two types of constraint in the error function were quantities that also had to be taken into consideration in order for the solution to be physically relevant. It would not have been good enough simply to fit the NIST pressure-volume data with no regard for the phase behaviour of the system.

In reality, we found that several runs of the fitting procedure with different values for W were needed to generate a feel for what would give a good balance, and find an acceptable compromise between fitting the two types of constraint for density and VLE fitting. We highlight that a value of W close to 0 meant the search algorithm would look more closely for parameter combinations that would fit the coexistence constraints, whilst a value of W close to 1 meant that it would instead prioritise pressure fitting the pressure data.

For the first guess using simulated annealing we eventually came to the realisation that it was important to set W quite high within the range 0 to 1 to take account of the fact that the pressure data must be accurately modelled in the first place in order for all the subsequent fittings to also be accurate: We felt a good pressure behaviour was slightly more fundamental to an accurate equation of state than phase behaviour at this stage of the development as correct phase behaviour can be inferred from pressure, but not the other way round. For example, setting $W = 0$ would remove the term for pressure considerations from Equation (4.1) and make the search algorithm look only for parameters that would yield a good VLE description. Conversely, setting $W = 1$ would remove the term for VLE considerations from Equation (4.1) and make the search algorithm look only for parameters that would yield a good pressure description. Bearing in mind the overall aims we set out for the model, specifically that it must give accurate descriptions for both density and VLE behaviours, we had to find the optimum value of W that would ensure a proportionate fit to both types of data. After some trial and error to determine this optimum value, we settled on a value of $W = 0.75$ for the very first fitting at the critical temperature, as this would allow the fitting regime to find parameters which would give a good performance in predicting the pressure whilst maintaining some consideration for the requirement to include a good phase behaviour prediction.

4.2 Generalising to Sub-Critical Temperatures

After the first set of parameters had been established for T_c , we moved our attention to a very slightly lower temperature (304K). Given that our aim was to build an idea of how the proposed EoS behaved at a range of temperatures up to and including T_c , we again sought to minimise the value of E over the set of seven parameters a to g at this new temperature, much as before. The significant difference in this fitting was that we would no longer be using simulated annealing, but the default local minimisation algorithm programmed into Mathematica as described in Chapter 2, where we would take as our starting point the set of parameter values determined

at the previous temperature point, in this case T_c . Our reason for this was that the local minimisation technique starts its search of the seven-dimensional space from a specified location, whereas simulated annealing does not. In this way we would be able to influence the search for the optimum set of parameters to look in a region of the space close to the region where the previous set of optimum parameters were found. This was beneficial because ultimately we would need to specify a temperature dependence for each of the model parameters, and if we could ensure that as the temperature varied so too would the value of the parameter in a smooth way, we might hope that the continuous nature of the physical behaviour might be borne out by smoothly varying parameters.

At sub-critical temperatures we again used the error function (4.1), this time with the constraints as given in Equations (3.3) to (3.5):

$$\Gamma = \left(\log \phi(v_{\text{DP}}) - \log \phi(v_{\text{BP}}) \right)^2 + \left(P(v, T) \Big|_{v=v_{\text{DP}}} - P_{\text{vap}} \right)^2 + \left(P(v, T) \Big|_{v=v_{\text{BP}}} - P_{\text{vap}} \right)^2. \quad (4.3)$$

Again, this allowed us to fully define the error function which the Mathematica local minimisation routine mentioned in Chapter 2 would be able to use in order to find the set of parameters at the new temperature which optimised our model.

In this way we repeated the process of fitting to the NIST data at a comprehensive range of temperatures below the critical temperature. We used the default local optimisation procedure for these steps and again after some experimentation to find a value for the weighting function, we found a value of $W = 0.01$ to usually work well, although while fitting at some temperatures we occasionally perturbed this slightly to affect either a smooth variation of the model parameters with temperature or a better balance between the pressure accuracy and predictions of VLE behaviour. Ultimately, our criterion for selecting a value for W was that the average percentage errors in predictions of the two types of behaviour should be similar. We note that at subsequent temperature fittings W took on a much lower value than the first time as a solution exhibiting a good pressure behaviour had been “locked in” by the initial stage where W was higher. Thus, we were free to look a little more closely at ensuring phase behaviour was accurately modelled.

4.3 Generalising to Super–Critical Temperatures

We note that fitting to temperatures above T_c was also possible in this set-up by setting

$$\Gamma = 0, \tag{4.4}$$

as there is no coexistence constraint to be enforced here, and using the error function as before. We note that the range of ambient temperatures found in the majority of locations where CCS is proposed (for example, Northern Europe), is expected to operate significantly below the supercritical temperatures (approximately 31°C and over), yet we extend our model to this elevated temperature range as it may prove to be a useful addition to the model, for example in describing behaviour in the latter stages of the pipeline transport process before the injection stage of CCS, which can sometimes occur at temperatures around 35°C, or at the exit of the compression stage where temperatures can reach 40–50°C.

4.4 Variation of Model Parameters with Respect to Temperature

We repeated this process at the many different temperature points in our intended region of fitting. We chose this to be from 260K and 335K, as we identified this to be a slightly wider temperature range than CCS pipelines could be expected to encounter, so by fitting to this range, bearing in mind the pressure range we had selected, we would ensure the model could be of use in any CCS pipeline scenario. We fit the parameter values obtained by the search routines to a function in T , thus allowing us to formulate a picture of how each parameter $a(T), b(T), \dots, g(T)$ varied continuously with temperature. This fully determined the equation of state, giving an expression for P in terms of just v and T . Having done this, we report in Table 4.1 the parameter values we found to optimise the system at each temperature. We wanted to ensure we had proposed a relevant temperature variation for each parameter, which would closely match the values in this table. In order to be able to employ some mathematical insight into this, we also present the values quoted in Table 4.1 graphically for each parameter. For example, values for parameter a_{CO_2} obtained through the sequential process of using simulated annealing and local minimisation at different temperatures as described above, where the subscript CO_2 denotes specifically that this value of parameter a corresponds to the pure carbon dioxide case, are shown for temperatures below T_c in Figure 4.1 and above T_c in a similar plot in Figure 4.2.

| $T(K)$ | a_{CO_2} | b_{CO_2} | c_{CO_2} | d_{CO_2} | e_{CO_2} | f_{CO_2} | g_{CO_2} |
|----------|------------|------------|------------|---------------|------------|------------|------------|
| 260 | 0.369524 | 0.367818 | 0.125183 | -0.000374 | 0.780747 | 0.098833 | 0.045463 |
| 265 | 0.363018 | 0.356758 | 0.127792 | -0.000374 | 0.780747 | 0.099351 | 0.045960 |
| 270 | 0.356738 | 0.345941 | 0.130935 | -0.000374 | 0.780747 | 0.100522 | 0.046091 |
| 273.15 | 0.353753 | 0.339103 | 0.133745 | -0.000374 | 0.780747 | 0.101314 | 0.046273 |
| 275 | 0.352635 | 0.334360 | 0.135155 | -0.000374 | 0.780747 | 0.100010 | 0.047680 |
| 278.15 | 0.349700 | 0.327409 | 0.138206 | -0.000374 | 0.780747 | 0.100852 | 0.047762 |
| 280 | 0.347979 | 0.323392 | 0.140225 | -0.000374 | 0.780747 | 0.101620 | 0.047543 |
| 285 | 0.343788 | 0.312494 | 0.146504 | -0.000374 | 0.780747 | 0.104030 | 0.046656 |
| 288.15 | 0.342452 | 0.304852 | 0.151022 | -0.000374 | 0.780747 | 0.103906 | 0.047526 |
| 290 | 0.341598 | 0.300542 | 0.154080 | -0.000374 | 0.780747 | 0.104501 | 0.047415 |
| 290.15 | 0.341531 | 0.300195 | 0.154336 | -0.000374 | 0.780747 | 0.104560 | 0.047408 |
| 291 | 0.334409 | 0.304063 | 0.162855 | -0.000374 | 0.780747 | 0.100603 | 0.050768 |
| 292 | 0.333988 | 0.301780 | 0.164693 | -0.000374 | 0.780747 | 0.100958 | 0.050712 |
| 293 | 0.333391 | 0.299669 | 0.166641 | -0.000374 | 0.780747 | 0.101837 | 0.050200 |
| 293.15 | 0.333442 | 0.299248 | 0.166944 | -0.000374 | 0.780747 | 0.101643 | 0.050411 |
| 294 | 0.333217 | 0.297275 | 0.168698 | -0.000374 | 0.780747 | 0.101877 | 0.050429 |
| 294.5 | 0.333293 | 0.295975 | 0.169781 | -0.000374 | 0.780747 | 0.101581 | 0.050826 |
| 295 | 0.332991 | 0.294970 | 0.170886 | -0.000374 | 0.780747 | 0.102211 | 0.050397 |
| 295.5 | 0.327151 | 0.298688 | 0.176698 | -0.000374 | 0.780747 | 0.100414 | 0.051963 |
| 296 | 0.327087 | 0.297534 | 0.177863 | -0.000374 | 0.780747 | 0.100485 | 0.052041 |
| 296.5 | 0.327160 | 0.296298 | 0.179083 | -0.000374 | 0.780747 | 0.100277 | 0.052370 |
| 297 | 0.327371 | 0.294982 | 0.180368 | -0.000374 | 0.780747 | 0.099785 | 0.052956 |
| 297.5 | 0.327344 | 0.293857 | 0.181672 | -0.000374 | 0.780747 | 0.099934 | 0.052965 |
| 298 | 0.327498 | 0.292628 | 0.183056 | -0.000374 | 0.780747 | 0.099714 | 0.053308 |
| 298.15 | 0.327501 | 0.292295 | 0.183478 | -0.000374 | 0.780747 | 0.099757 | 0.053310 |
| 298.5 | 0.327488 | 0.291539 | 0.184468 | -0.000374 | 0.780747 | 0.099972 | 0.053217 |
| 299 | 0.327705 | 0.290322 | 0.185984 | -0.000374 | 0.780747 | 0.099769 | 0.053546 |
| 299.5 | 0.327841 | 0.289195 | 0.187556 | -0.000374 | 0.780747 | 0.099864 | 0.053600 |
| 300 | 0.316831 | 0.297393 | 0.196327 | -0.000374 | 0.780747 | 0.096801 | 0.056346 |
| 300.5 | 0.317132 | 0.296246 | 0.198061 | -0.000374 | 0.780747 | 0.096403 | 0.056870 |
| 301 | 0.317278 | 0.295254 | 0.199853 | -0.000374 | 0.780747 | 0.096562 | 0.056878 |
| 301.5 | 0.317632 | 0.294200 | 0.201836 | -0.000374 | 0.780747 | 0.096365 | 0.057214 |
| 302 | 0.317896 | 0.293291 | 0.203947 | -0.000374 | 0.780747 | 0.096660 | 0.057086 |
| 302.5 | 0.318518 | 0.292290 | 0.206393 | -0.000374 | 0.780747 | 0.096350 | 0.057516 |
| 303 | 0.315041 | 0.294811 | 0.211153 | -0.000374 | 0.780747 | 0.095212 | 0.058670 |
| 303.15 | 0.315262 | 0.294589 | 0.212058 | -0.000374 | 0.780747 | 0.095178 | 0.058740 |
| 303.5 | 0.315713 | 0.294227 | 0.214359 | -0.000374 | 0.780747 | 0.095333 | 0.058680 |
| 304 | 0.229488 | 0.361051 | 0.236202 | -0.000374 | 0.780747 | 0.091201 | 0.062049 |
| 304.1282 | 0.271294 | 0.332617 | 0.238762 | -0.000374 | 0.780747 | 0.078770 | 0.074028 |
| 304.5 | 0.220559 | 0.357053 | 0.217490 | -5.384474E-13 | 0.780747 | 0.104931 | 0.050584 |
| 305 | 0.220559 | 0.357053 | 0.217490 | -5.384474E-13 | 0.780747 | 0.104931 | 0.050584 |
| 305.5 | 0.220559 | 0.357053 | 0.217490 | -5.384474E-13 | 0.780747 | 0.104931 | 0.050584 |
| 306 | 0.220559 | 0.357053 | 0.217490 | -5.384474E-13 | 0.780747 | 0.104931 | 0.050584 |
| 306.5 | 0.218855 | 0.354471 | 0.219015 | -2.692236E-13 | 0.780747 | 0.106345 | 0.049896 |
| 307 | 0.218226 | 0.353668 | 0.219518 | -2.692236E-13 | 0.780747 | 0.106846 | 0.049642 |
| 307.5 | 0.218226 | 0.353668 | 0.219518 | -2.692236E-13 | 0.780747 | 0.106846 | 0.049642 |
| 308 | 0.218226 | 0.353668 | 0.219518 | -2.692236E-13 | 0.780747 | 0.106846 | 0.049642 |
| 308.5 | 0.215691 | 0.351925 | 0.221185 | -2.692236E-13 | 0.780747 | 0.108419 | 0.048817 |
| 309 | 0.214702 | 0.351501 | 0.221777 | -2.687911E-13 | 0.780747 | 0.108962 | 0.048525 |
| 309.5 | 0.213678 | 0.351120 | 0.222378 | -2.292181E-13 | 0.780747 | 0.109514 | 0.048224 |
| 310 | 0.212633 | 0.350769 | 0.222983 | -2.292181E-13 | 0.780747 | 0.110075 | 0.047917 |
| 310.5 | 0.212633 | 0.350769 | 0.222983 | -2.292181E-13 | 0.780747 | 0.110075 | 0.047917 |
| 311 | 0.210520 | 0.350117 | 0.224197 | -2.292181E-13 | 0.780747 | 0.111223 | 0.047278 |
| 311.5 | 0.209466 | 0.349802 | 0.224803 | -1.954713E-13 | 0.780747 | 0.111809 | 0.046948 |
| 312 | 0.209466 | 0.349802 | 0.224803 | -1.954713E-13 | 0.780747 | 0.111809 | 0.046948 |
| 312.5 | 0.207387 | 0.349168 | 0.226006 | -1.954712E-13 | 0.780747 | 0.113005 | 0.046267 |
| 313 | 0.206369 | 0.348843 | 0.226603 | -1.954712E-13 | 0.780747 | 0.113615 | 0.045916 |
| 313.5 | 0.206369 | 0.348843 | 0.226603 | -1.954712E-13 | 0.780747 | 0.113615 | 0.045916 |
| 314 | 0.203427 | 0.347799 | 0.228363 | -1.954711E-13 | 0.780747 | 0.115495 | 0.044820 |
| 314.5 | 0.202490 | 0.347421 | 0.228938 | -1.954709E-13 | 0.780747 | 0.116138 | 0.044439 |
| 315 | 0.201577 | 0.347026 | 0.229507 | -1.954708E-13 | 0.780747 | 0.116791 | 0.044050 |
| 316 | 0.199829 | 0.346174 | 0.230626 | -3.909416E-14 | 0.780747 | 0.118125 | 0.043248 |
| 317 | 0.198190 | 0.345232 | 0.231715 | -1.954708E-14 | 0.780747 | 0.119498 | 0.042411 |
| 318 | 0.196666 | 0.344191 | 0.232774 | -1.954708E-14 | 0.780747 | 0.120914 | 0.041536 |
| 319 | 0.195259 | 0.343044 | 0.233802 | -1.954708E-14 | 0.780747 | 0.122373 | 0.040622 |
| 320 | 0.193968 | 0.341788 | 0.234800 | -1.954708E-14 | 0.780747 | 0.123877 | 0.039669 |
| 325 | 0.189045 | 0.333994 | 0.239438 | -1.954708E-14 | 0.780747 | 0.132034 | 0.034325 |
| 330 | 0.185791 | 0.324454 | 0.243890 | -1.954708E-14 | 0.780747 | 0.141024 | 0.028211 |
| 335 | 0.183236 | 0.314125 | 0.248578 | -1.954708E-14 | 0.780747 | 0.150615 | 0.021512 |

Table 4.1: Parameter values for pure carbon dioxide at each temperature

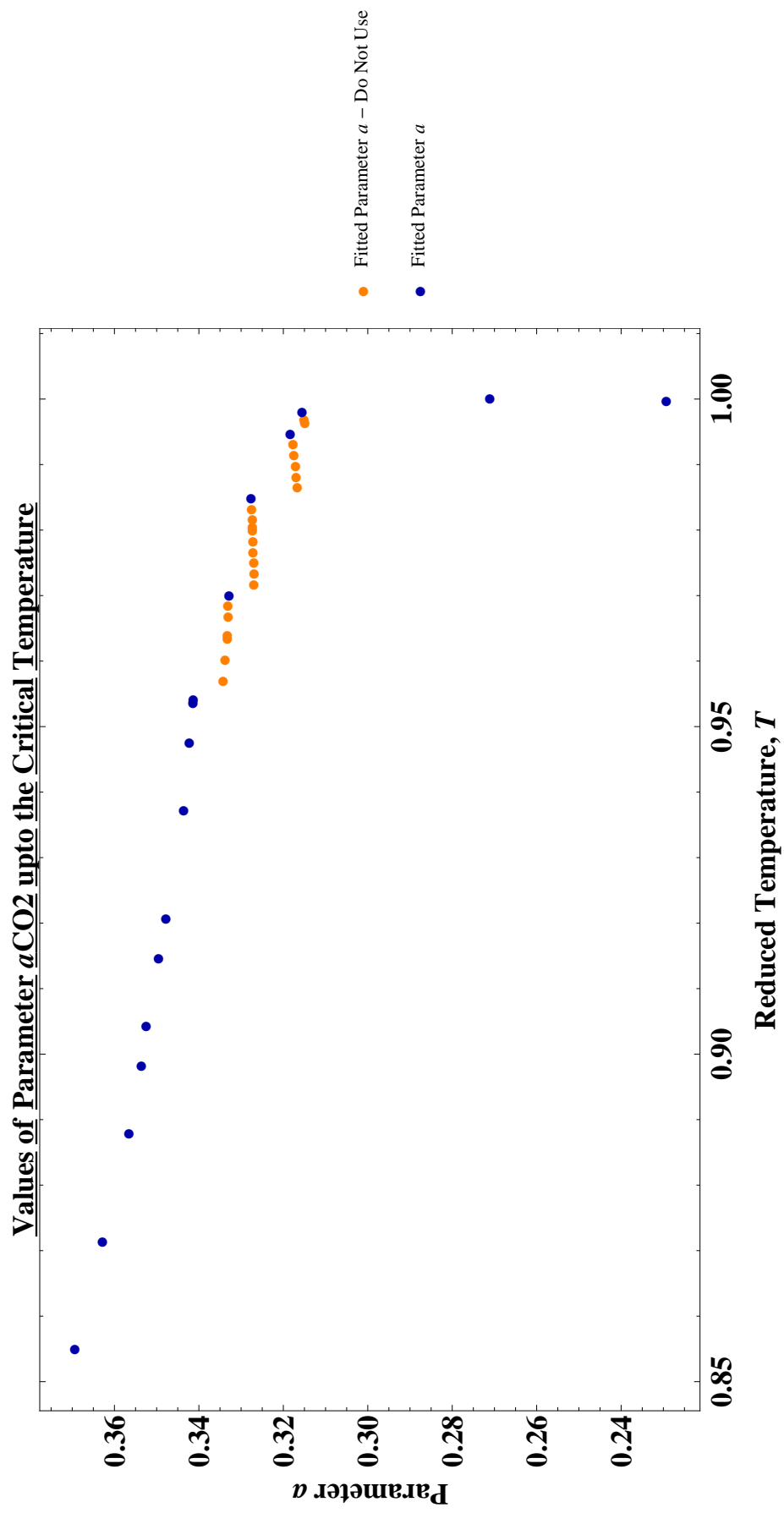


Figure 4.1: Values of parameter a_{CO_2} at sub-critical temperatures

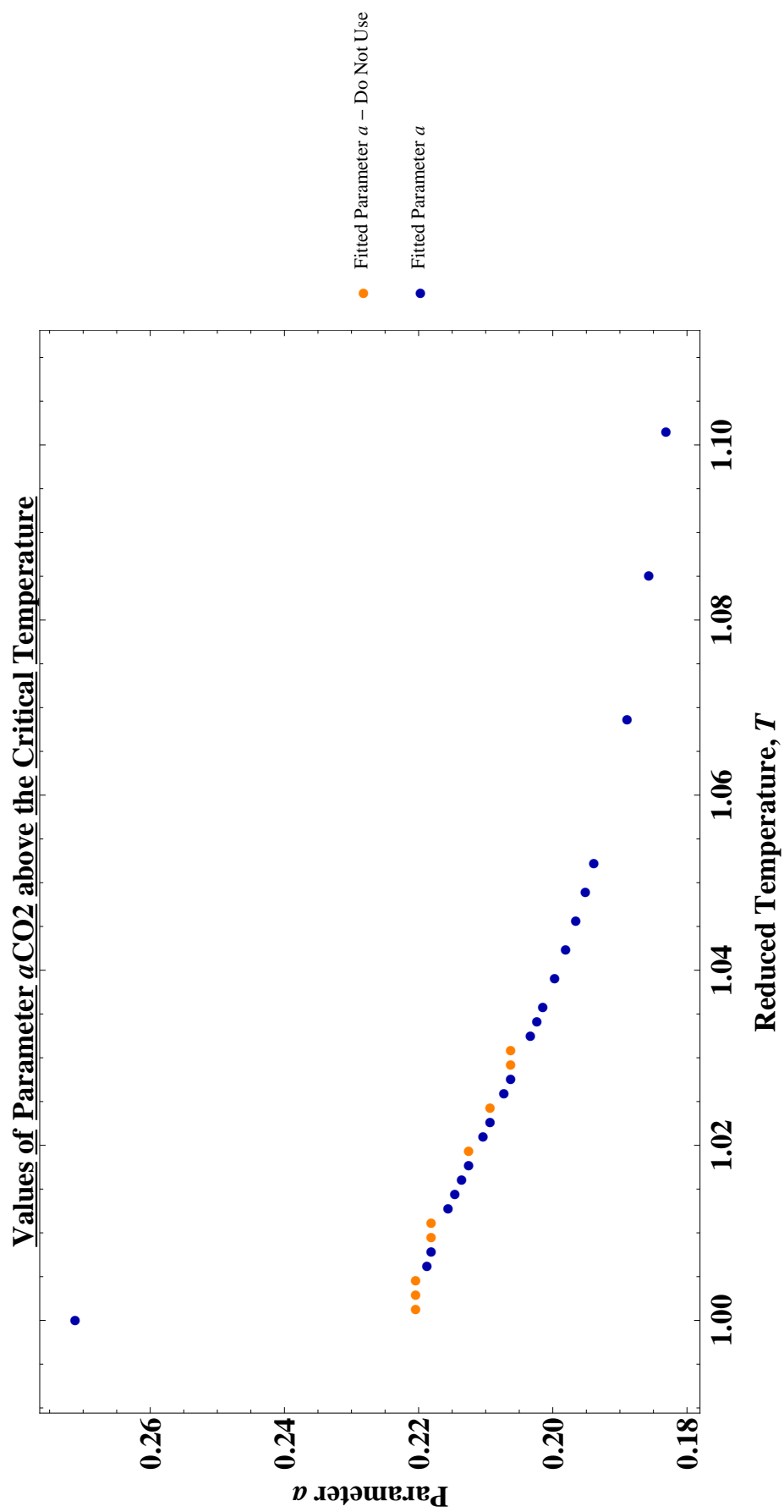


Figure 4.2: Values of parameter a_{CO_2} at super-critical temperatures for pure carbon dioxide

The orange markers in Figures 4.1 and 4.2 were those values of parameter a_{CO_2} which were seen not to obey the overall trend of the other parameter values throughout the temperature range (hence the legend identifies that these were not to be used). In the original fitting steps we could have compensated for this by altering the value of W where necessary, as detailed previously. This would have allowed all the points to align in a smooth way, but we skipped the step of actually doing this, instead discarding those points for which this would need to be done, and moving straight to the second-stage fitting of each parameter with T , as it would potentially have been a time consuming process to find the exact value of W which gave this good alignment, and we would have arrived at the same conclusion anyway. The end result that we would have a smooth curve for the temperature dependence of each parameter would have been the same if we neglected those values at this stage and fit without them.

We wished to have each parameter vary smoothly with T up to, including, and beyond the critical temperature, but we observed from Figures 4.1 and 4.2 what appears to be behaviour resembling a non-analytic variation of a_{CO_2} with T , as T_c was approached from either side. Taking inspiration from the Frobenius Method for series solutions close to singular points, where the gradient can become very steep, we suggested the following general form for each parameter in the pure CO_2 case for our model:

$$a_{\text{var}}(T; a_1, a_2, a_3, a_4) = |T - 1|^{a_1} (a_2 |T - 1|^2 + a_3 |T - 1| + a_4) + a_{\text{FIT}}(T_c), \quad (4.5)$$

where $a_{\text{FIT}}(T_c)$ was the exact value given in Table 4.1 determined in the fitting stages. This would ensure an excellent prediction of the critical point. We again established an error function similar in construction to the that in Equation (4.1):

$$\Gamma_a = \sum_{\text{all } T} (a_{\text{FIT}}(T) - a_{\text{var}}(T))^2, \quad (4.6)$$

where $a_{\text{FIT}}(T)$ is the value for parameter a given in Table 4.1 and $a_{\text{var}}(T; a_1, a_2, a_3, a_4)$ is the form of temperature dependence we assigned to parameter a in (4.5). We then minimised this using simulated annealing to find numerical values for a_1 to a_4 , thus giving us the complete temperature variation of a with T . This process was carried out twice; once below the critical temperature and once above, each time anchoring the variation at the critical temperature to the value given in Table 4.1, in doing so ensuring an excellent prediction of the critical point and a continuous (albeit non-differentiable at T_c) form for the parameter.

Our final derived expression for the parameter a , both below and above T_c , obtained using this method, was,

$$a_{\text{CO}_2}(T) = \begin{cases} |T - 1|^{0.626207}(33.9261|T - 1|^2 - 8.10461|T - 1| \\ + 0.805812) + 0.27129411630837575312 & T \leq 1 \\ |T - 1|^{5.514209492375366\text{E-}9}(3.556|T - 1|^2 - 0.765078|T - 1| \\ - 0.0467569) + 0.27129411630837575312 & T \geq 1 \end{cases} \quad (4.7)$$

a plot of which in the region of interest is as shown in Figure 4.3. We carried out exactly the same process to determine the other six parameters $b_{\text{CO}_2}(T) - g_{\text{CO}_2}(T)$. Below the critical temperature, b took values as demonstrated in Figure 4.1 and above the critical temperature as shown in Figure 4.5.

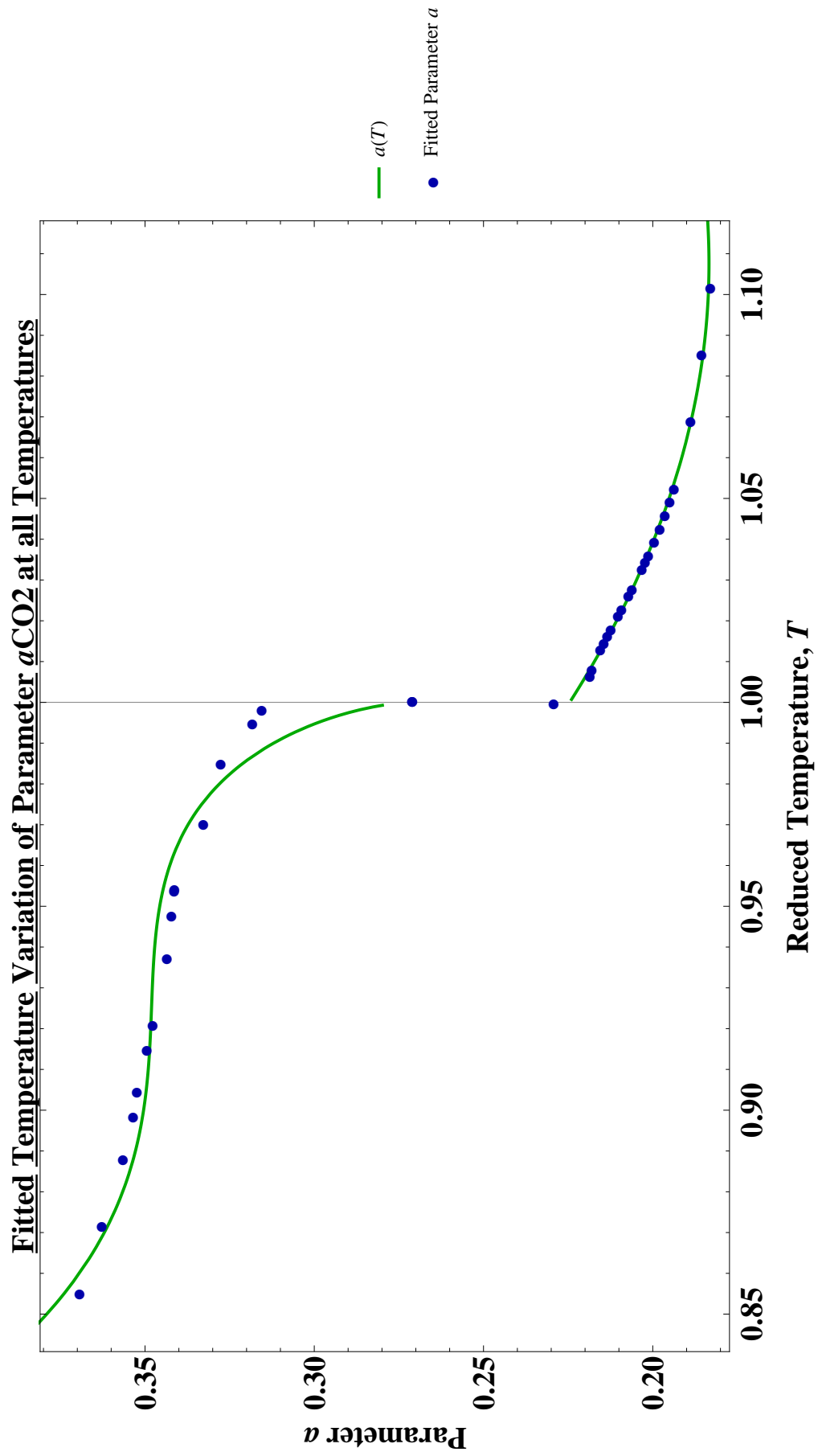


Figure 4.3: Variation of parameter a_{CO_2} at all temperatures

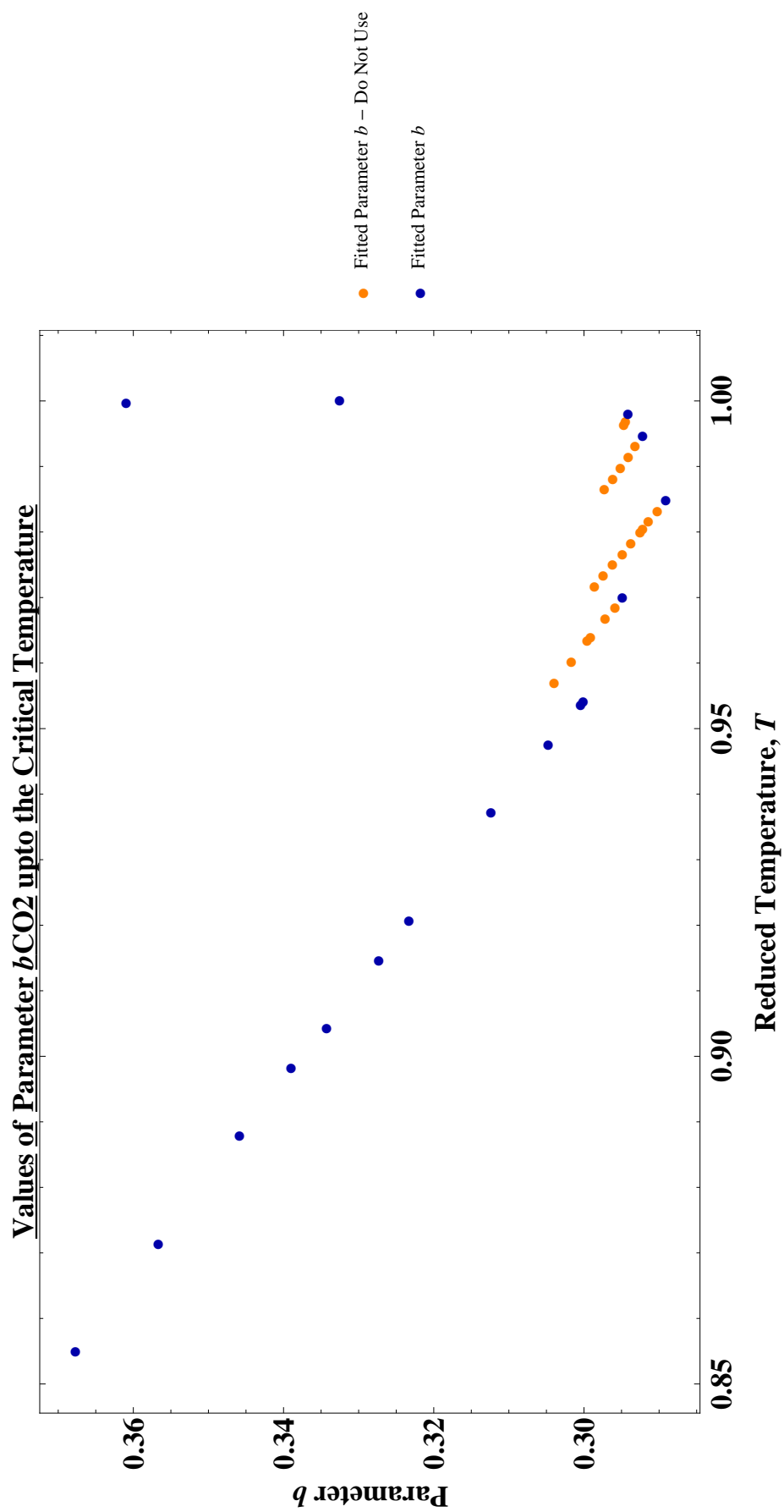


Figure 4.4: Values of parameter b_{CO_2} at sub-critical temperatures for pure carbon dioxide

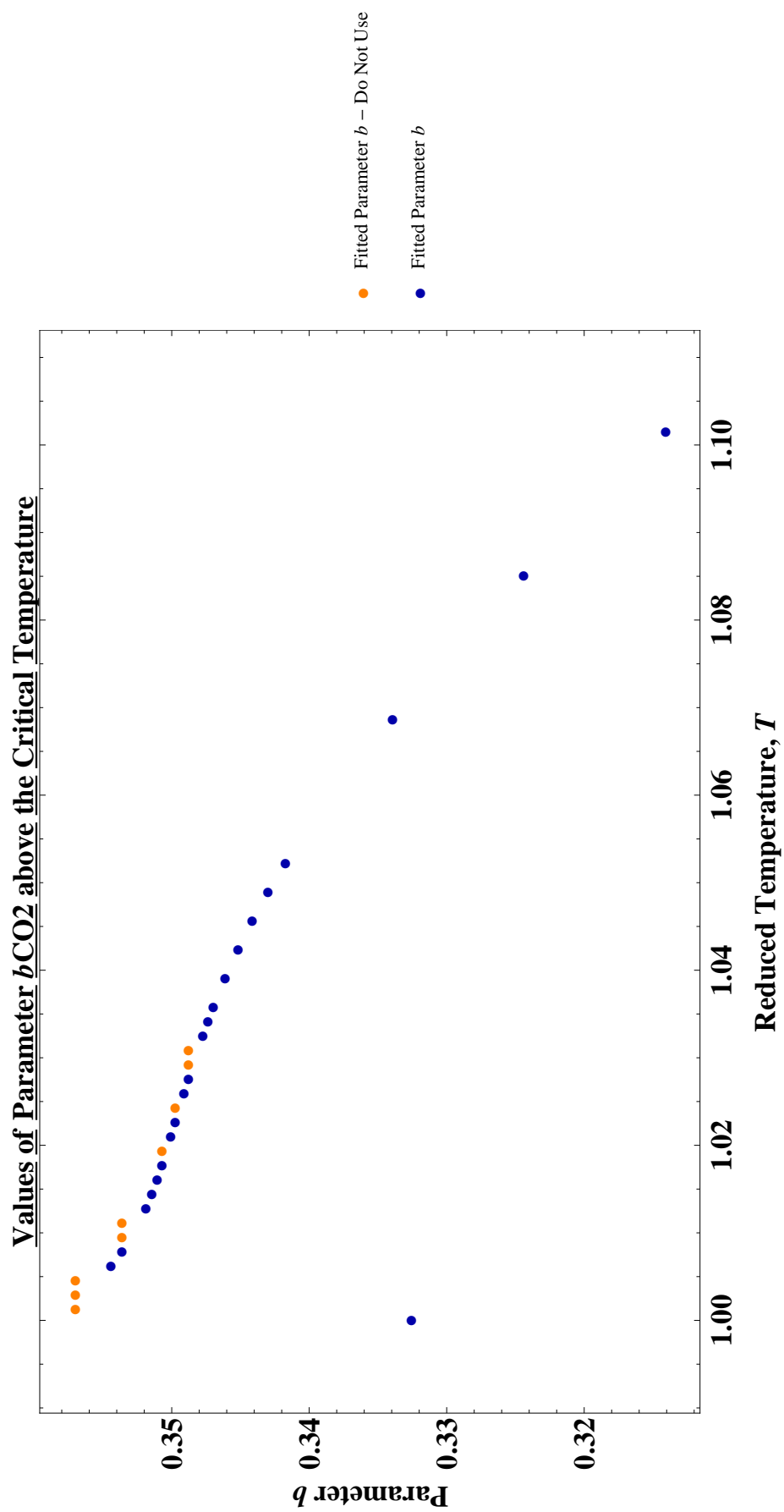


Figure 4.5: Values of parameter b_{CO_2} at super-critical temperatures for pure carbon dioxide

We again specified a functional form for b_{CO_2} in the same way as for a_{CO_2} :

$$b_{\text{var}}(T; b_1, b_2, b_3, b_4) = |T - 1|^{b_1} (b_2 |T - 1|^2 + b_3 |T - 1| + b_4) + b_{\text{FIT}}(T_c), \quad (4.8)$$

and upon minimising an analogous error function to that shown in Equation (4.6), obtained the following temperature definition for b_{CO_2} :

$$b_{\text{CO}_2}(T) = \begin{cases} |T - 1|^{0.405254} (-13.5708 |T - 1|^2 + 4.48534 |T - 1| - 0.295229) \\ \quad + 0.33261690686926754767 & T \leq 1 \\ |T - 1|^{5.5792801817977416\text{E-}9} (-3.07866 |T - 1|^2 - 0.0767956 |T - 1| \\ \quad + 0.0210443) + 0.33261690686926754767 & T \geq 1 \end{cases} \quad (4.9)$$

a plot of which is shown in Figure 4.6.

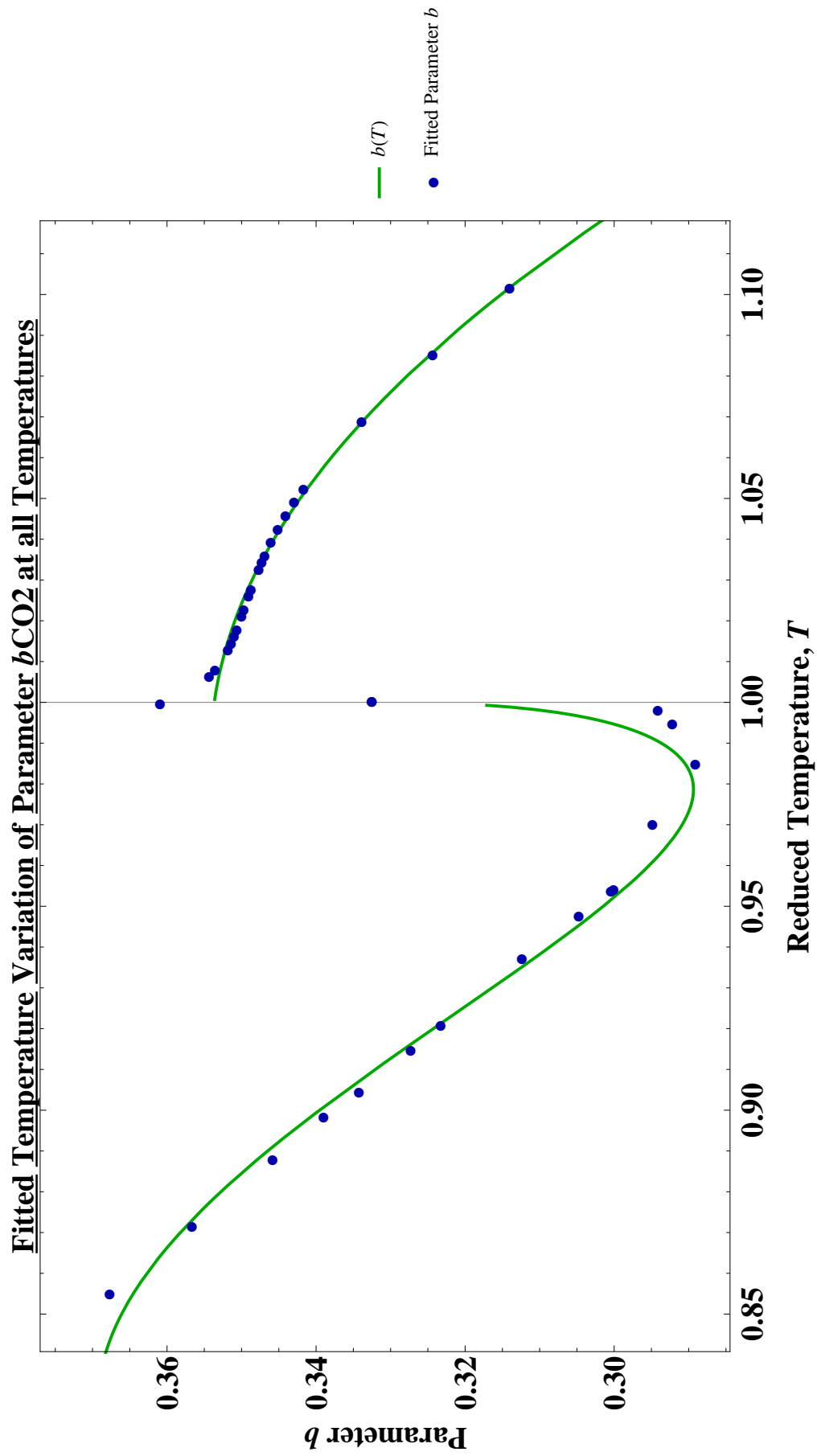


Figure 4.6: Variation of parameter b_{CO_2} at all temperatures in the CCS pipeline relevant range

For the remaining pure carbon dioxide parameters $c_{\text{CO}_2}(T)$ through to $g_{\text{CO}_2}(T)$, we carried out the same process, noting the slightly more complicated behaviour for parameter d in Figure 4.9, where we increased the order of the temperature dependence by one, and the minuscule variation of e with respect to T , where we opted for a different approach for this parameter, instead defining it to be take on a constant value; that being taken at the critical temperature.

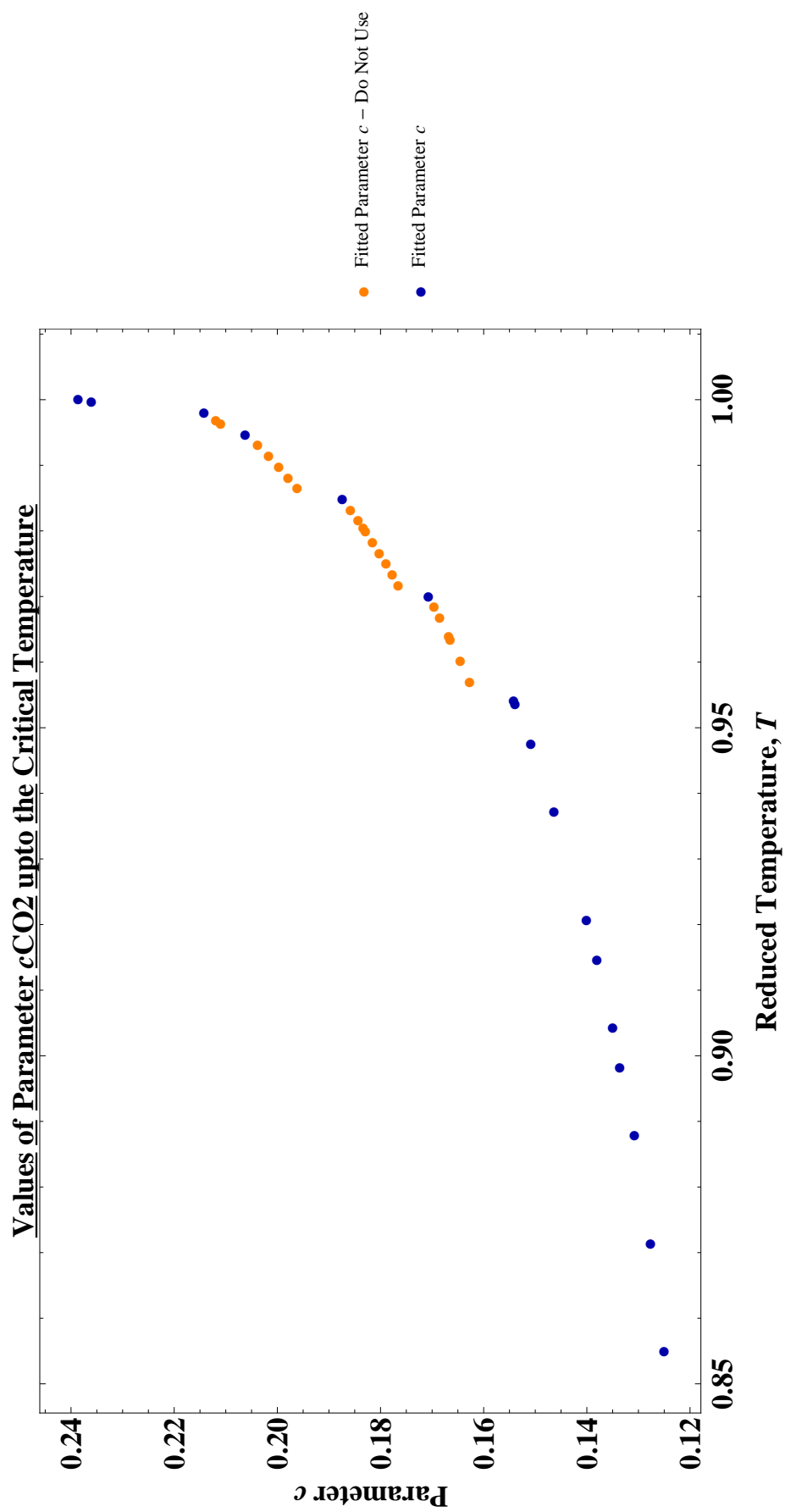


Figure 4.7: Values of parameter c_{CO_2} at sub-critical temperatures for pure carbon dioxide

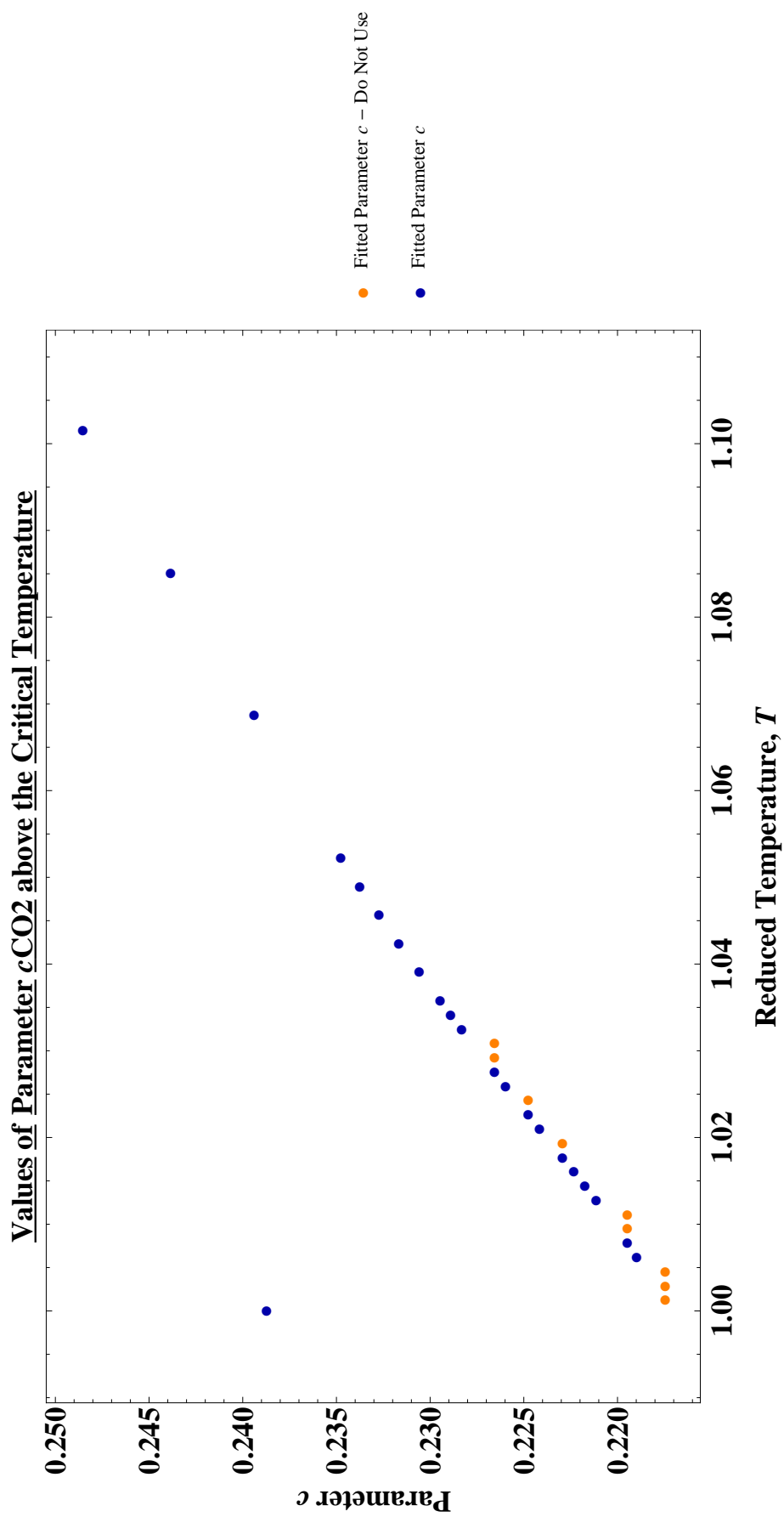


Figure 4.8: Values of parameter c_{CO_2} at super-critical temperatures for pure carbon dioxide

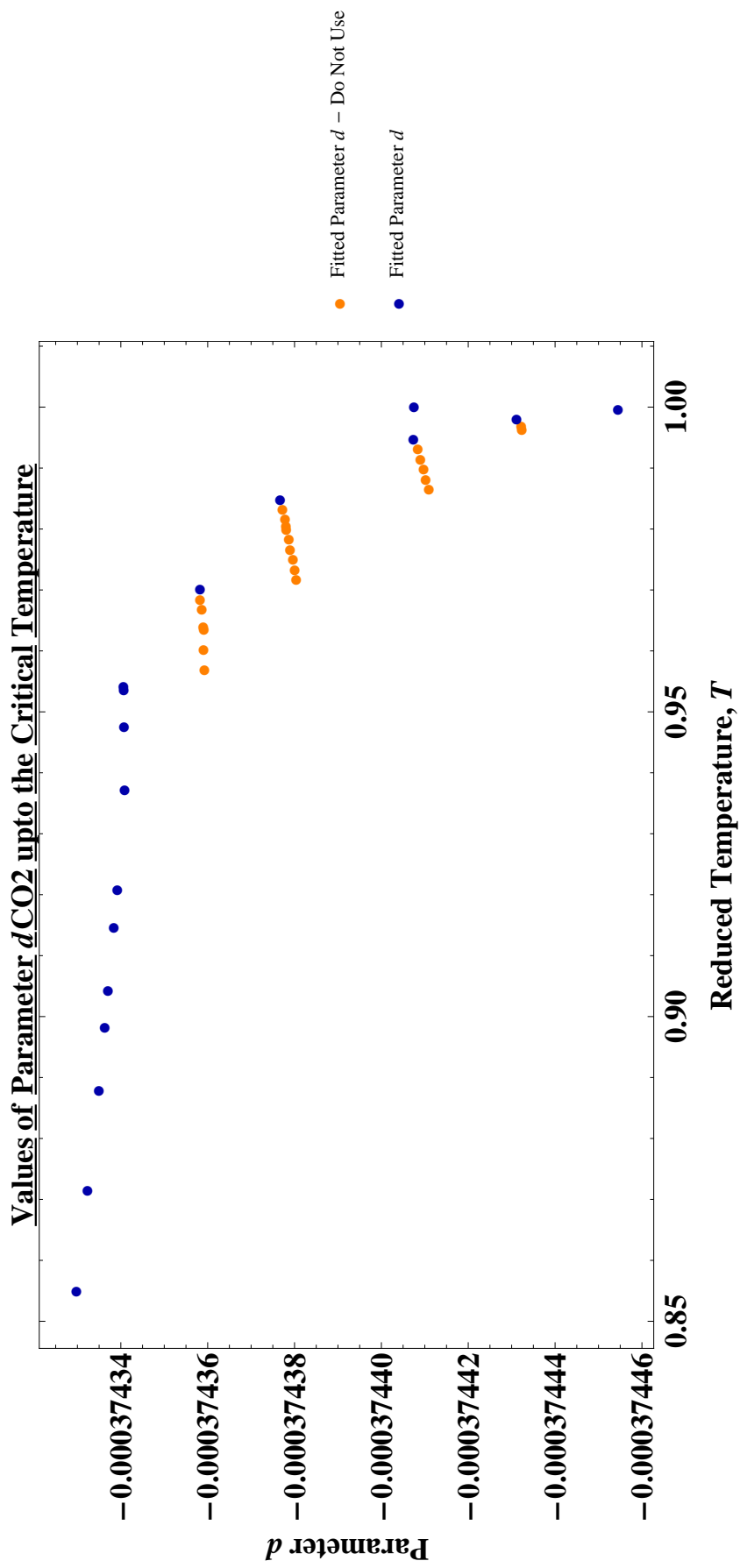


Figure 4.9: Values of parameter d_{CO_2} at sub-critical temperatures for pure carbon dioxide

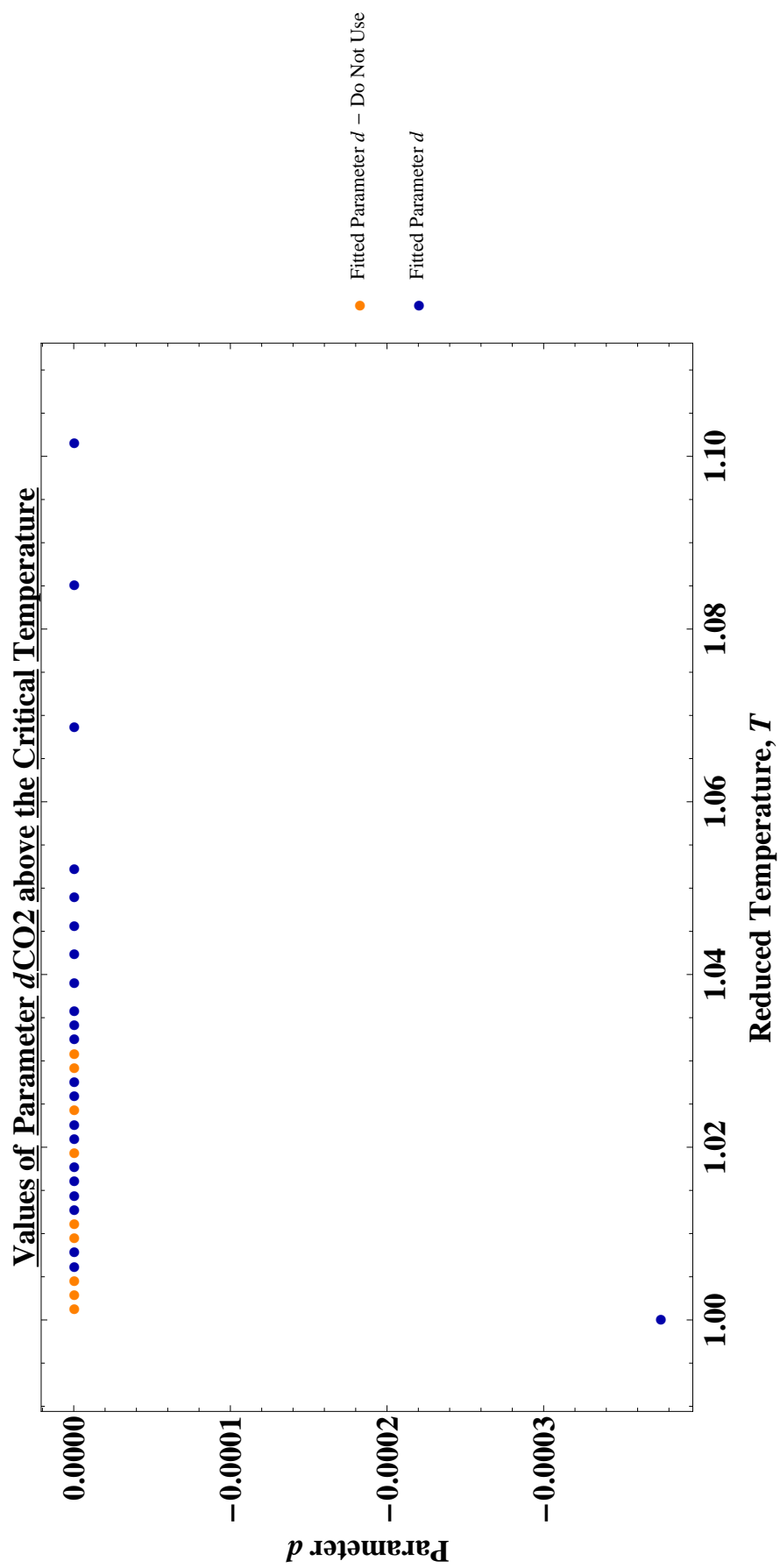


Figure 4.10: Values of parameter d_{CO_2} at super-critical temperatures for pure carbon dioxide

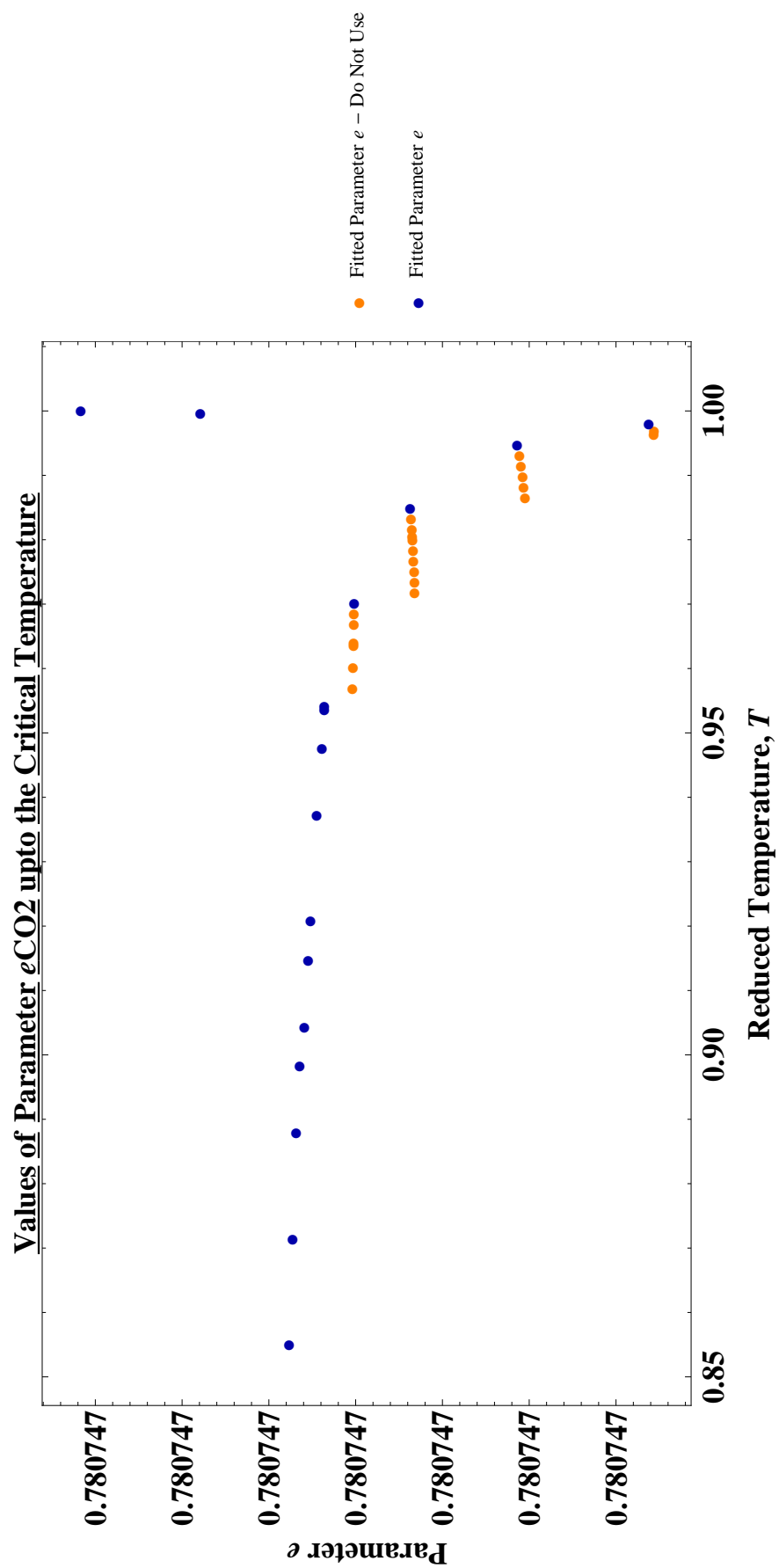


Figure 4.11: Variation of parameter e_{CO_2} at sub-critical temperatures for pure carbon dioxide

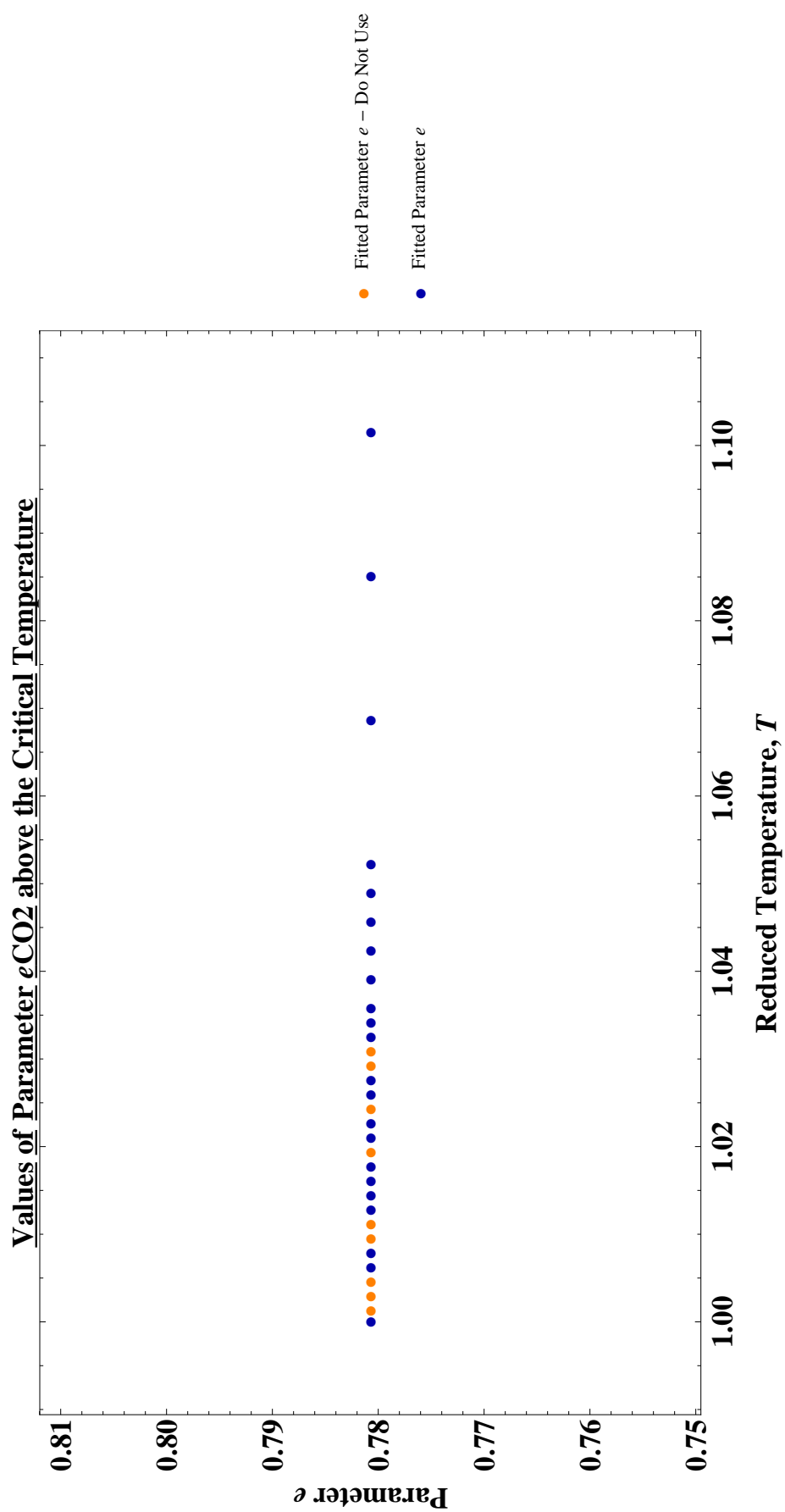


Figure 4.12: Values of parameter e_{CO_2} at super-critical temperatures for pure carbon dioxide

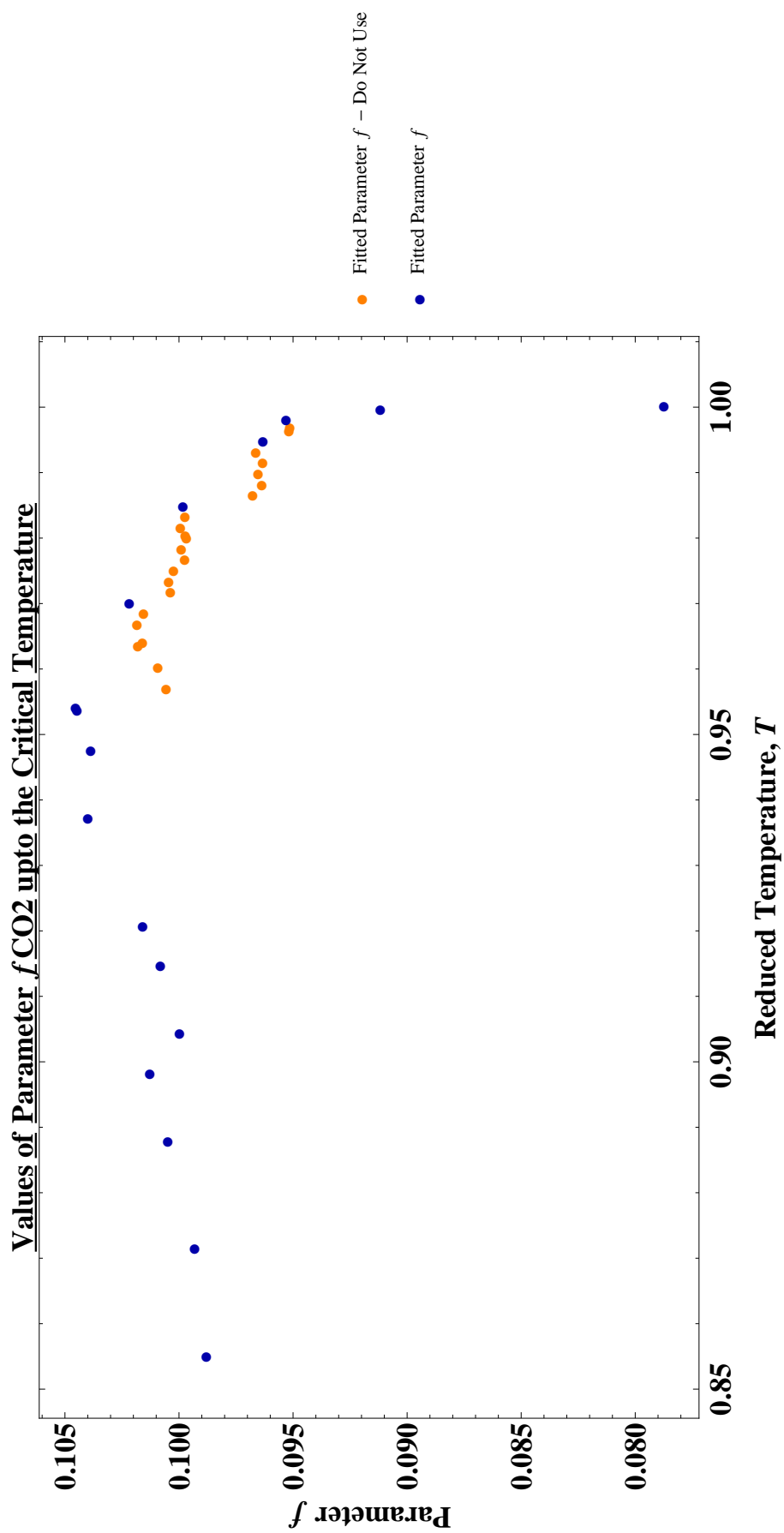


Figure 4.13: Values of parameter f_{CO_2} at sub-critical temperatures for pure carbon dioxide

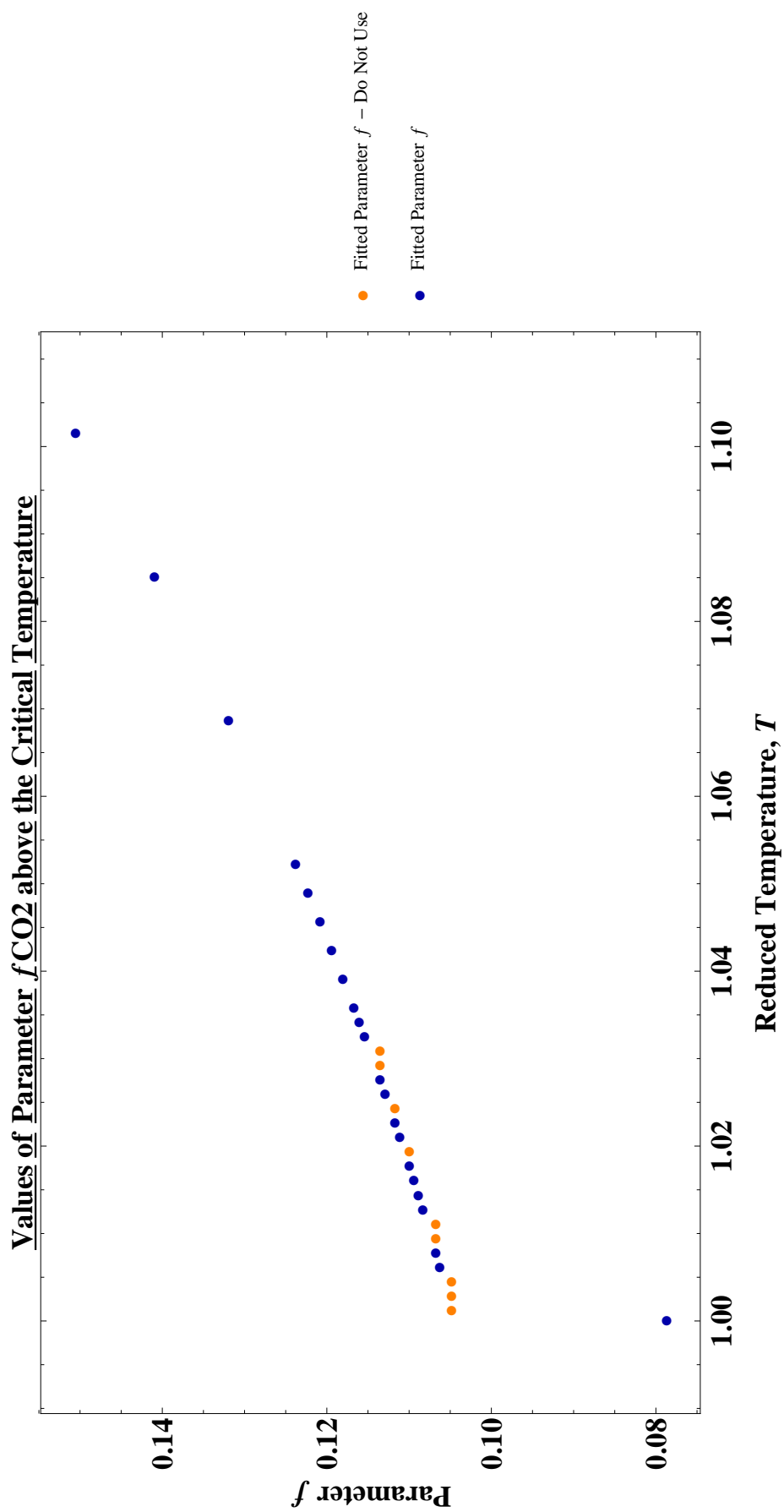


Figure 4.14: Values of parameter f_{CO_2} at super-critical temperatures for pure carbon dioxide

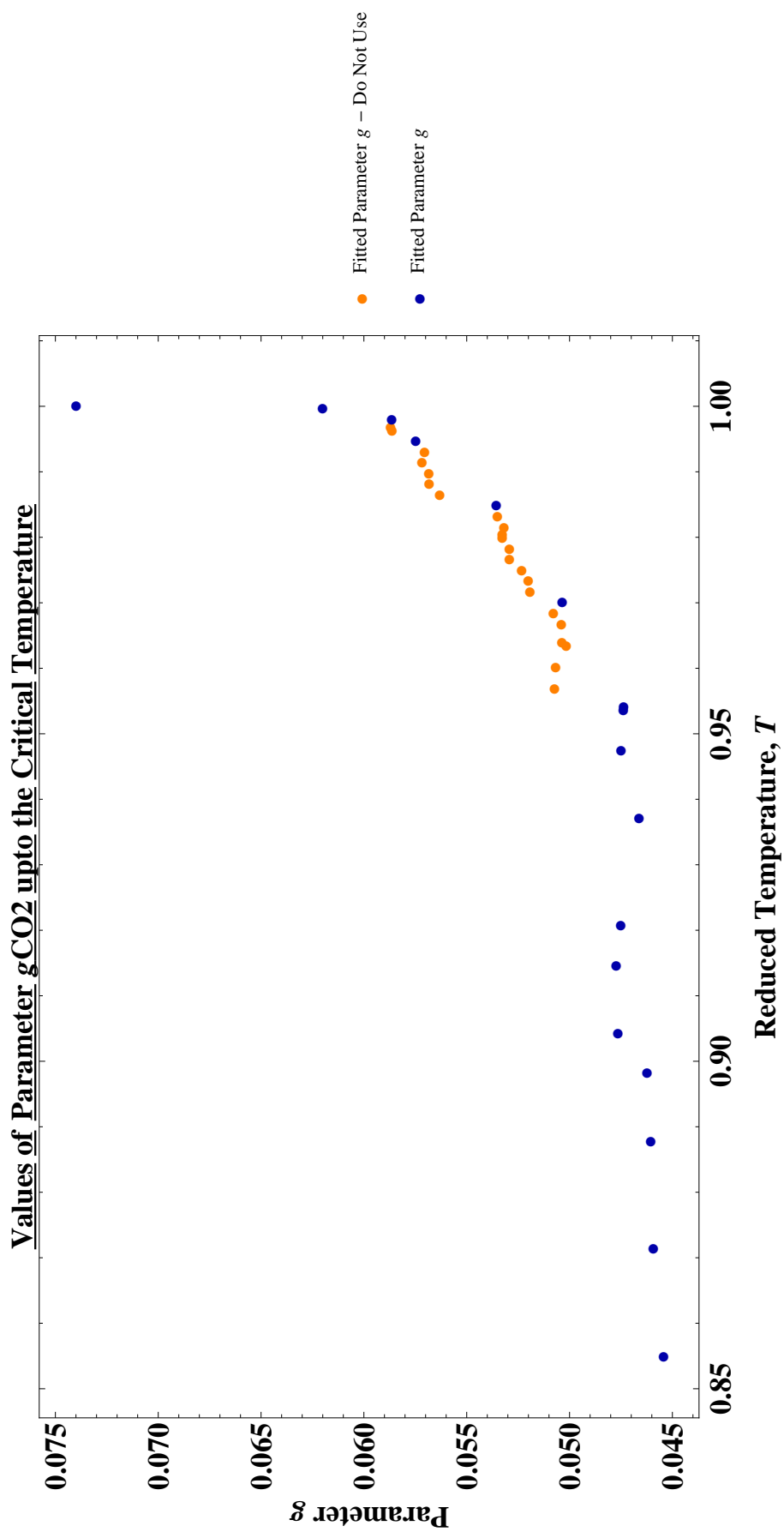
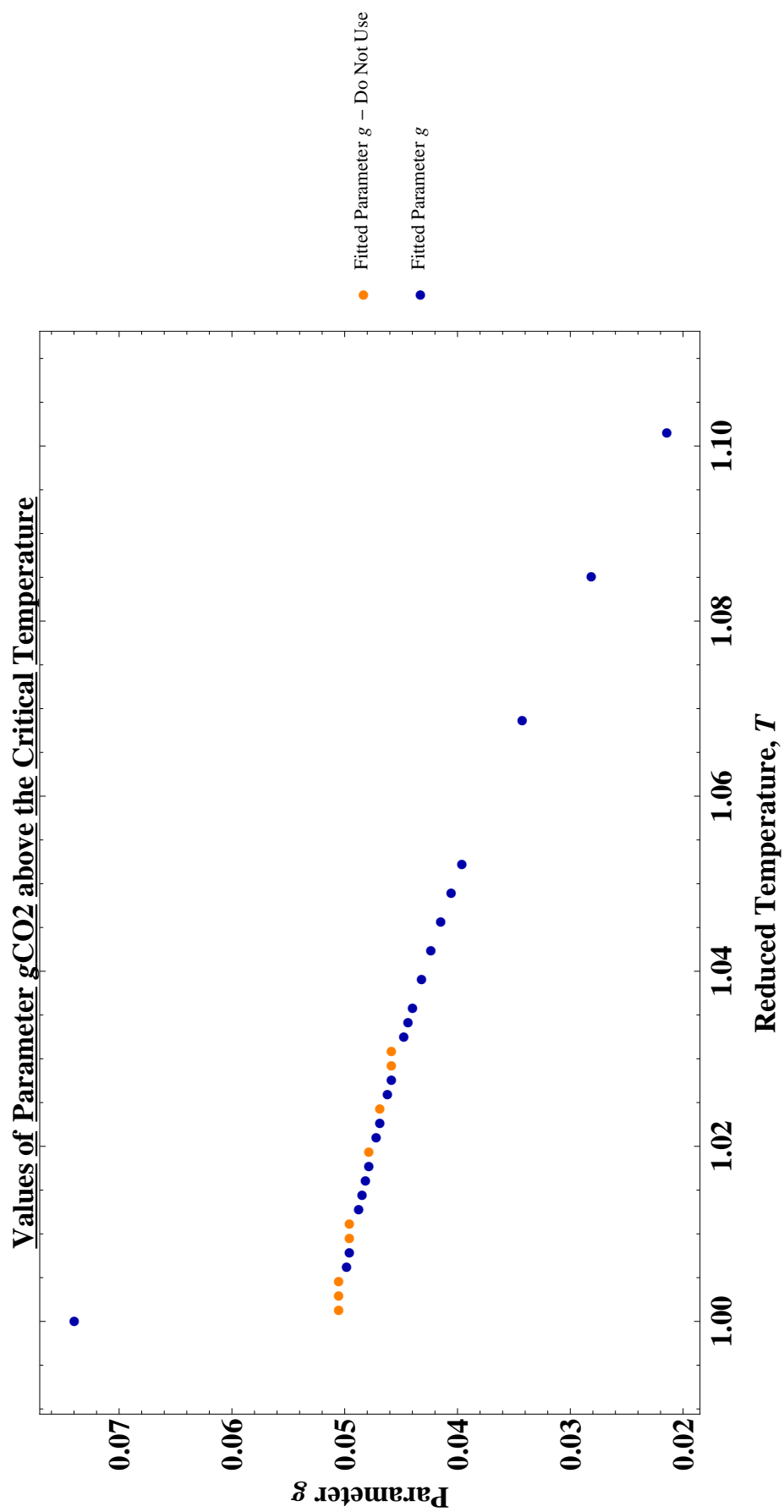


Figure 4.15: Values of parameter g_{CO_2} at sub-critical temperatures for pure carbon dioxide



$$c(T) = \begin{cases} |T-1|^{0.515789}(-3.77054|T-1|^2 + 1.72673|T-1| \\ - 0.478733) + 0.23876225996324883019 & T \leq 1 \\ |T-1|^{0.00608516}(-0.823306|T-1|^2 + 0.405298|T-1| \\ - 0.0229758) + 0.23876225996324883019 & T \geq 1 \end{cases} \quad (4.10)$$

$$d(T) = \begin{cases} |T-1|^{1.27068}(0.000634507|T-1|^3 - 8.327888244017052\text{E-}6|T-1|^2 \\ - 0.0000382867|T-1| + 4.661593764290955\text{E-}6) + \\ - 0.00037440735502740741443 & T \leq 1 \\ 0.000374402|T-1|^{4.7618206193929816\text{E-}7} + \\ - 0.00037440735502740741443 & T \geq 1 \end{cases} \quad (4.11)$$

$$e(T) = 0.78074651436175671059, \quad (4.12)$$

$$f(T) = \begin{cases} |T-1|^{0.192269}(0.210429|T-1|^2 - 0.199813|T-1| \\ + 0.0528131) + 0.078770114175749938219 & T \leq 1 \\ |T-1|^{6.022611289345914\text{E-}9}(1.7061|T-1|^2 + 0.281852|T-1| \\ + 0.0257812) + 0.078770114175749938219 & T \geq 1 \end{cases} \quad (4.13)$$

$$g(T) = \begin{cases} |T-1|^{0.198411}(-0.185594|T-1|^2 + 0.0931741|T-1| \\ - 0.0510056) + 0.074028115340316985540 & T \leq 1 \\ |T-1|^{2.1304304817762944\text{E-}9}(-1.51507|T-1|^2 - 0.135147|T-1| \\ - 0.0232326) + 0.074028115340316985540 & T \geq 1 \end{cases} \quad (4.14)$$

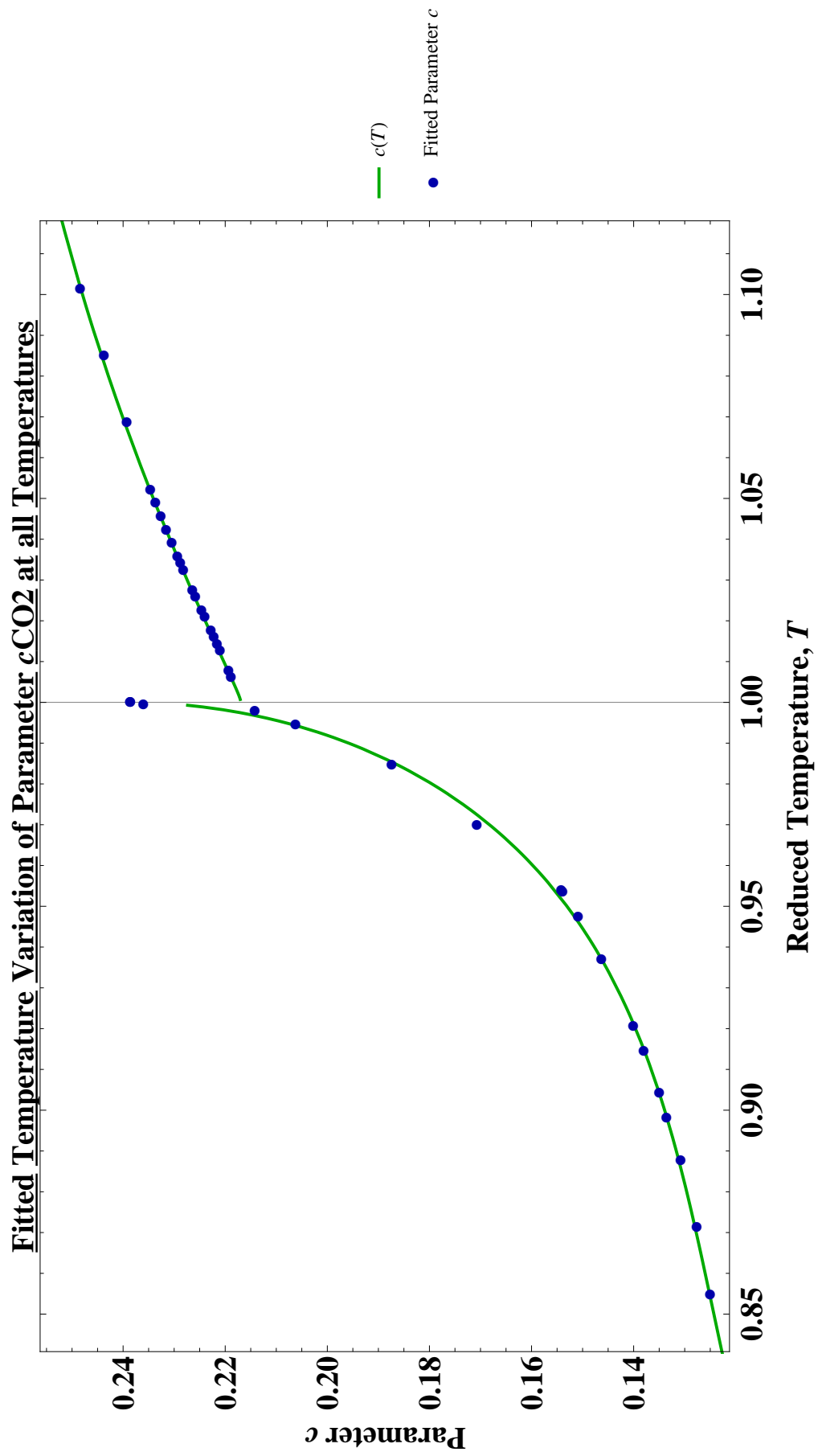


Figure 4.17: Variation of parameter c_{CO_2} at all temperatures in the CCS pipeline relevant range

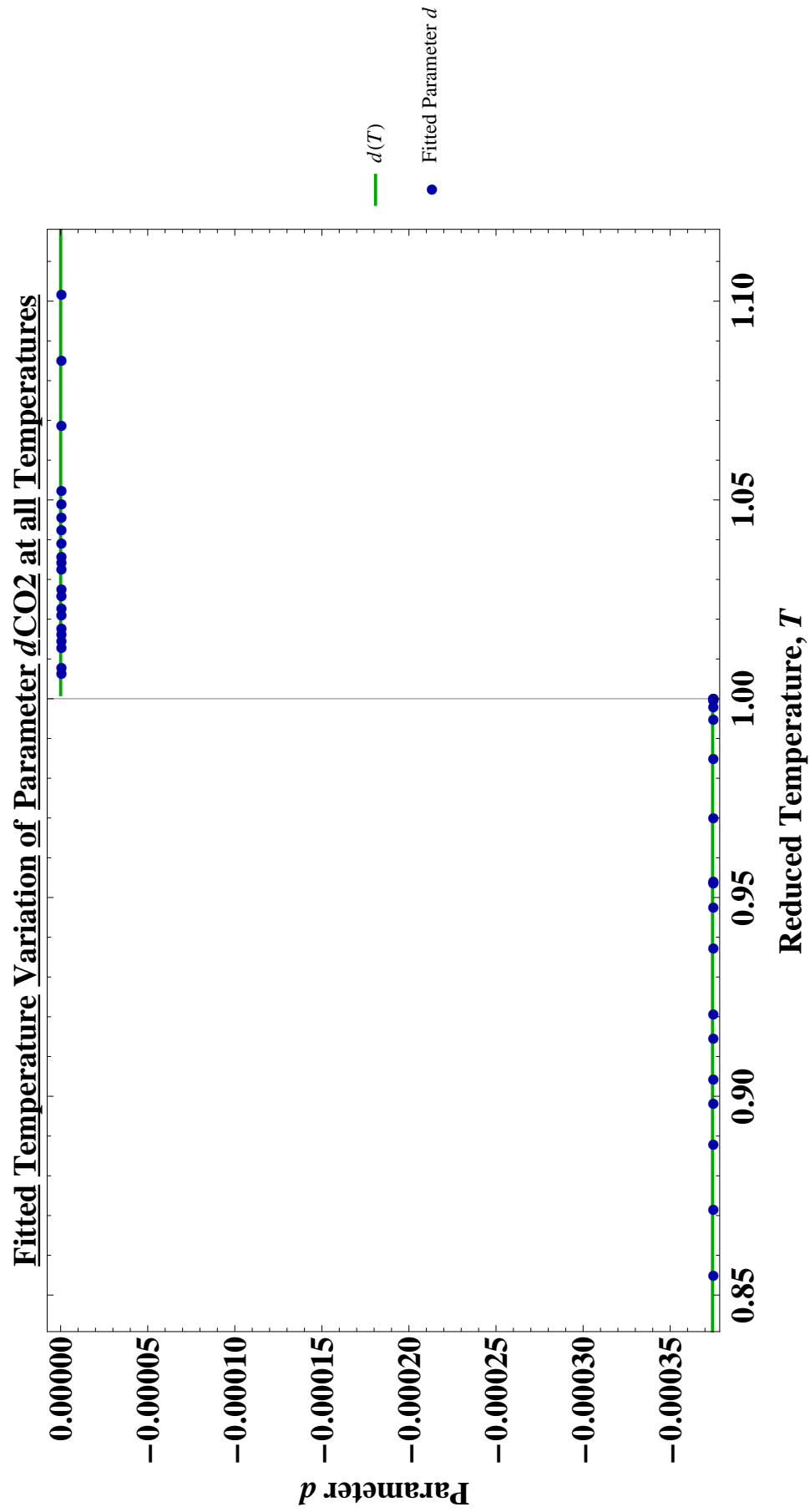


Figure 4.18: Values of parameter d_{CO_2} at sub-critical temperatures for pure carbon dioxide

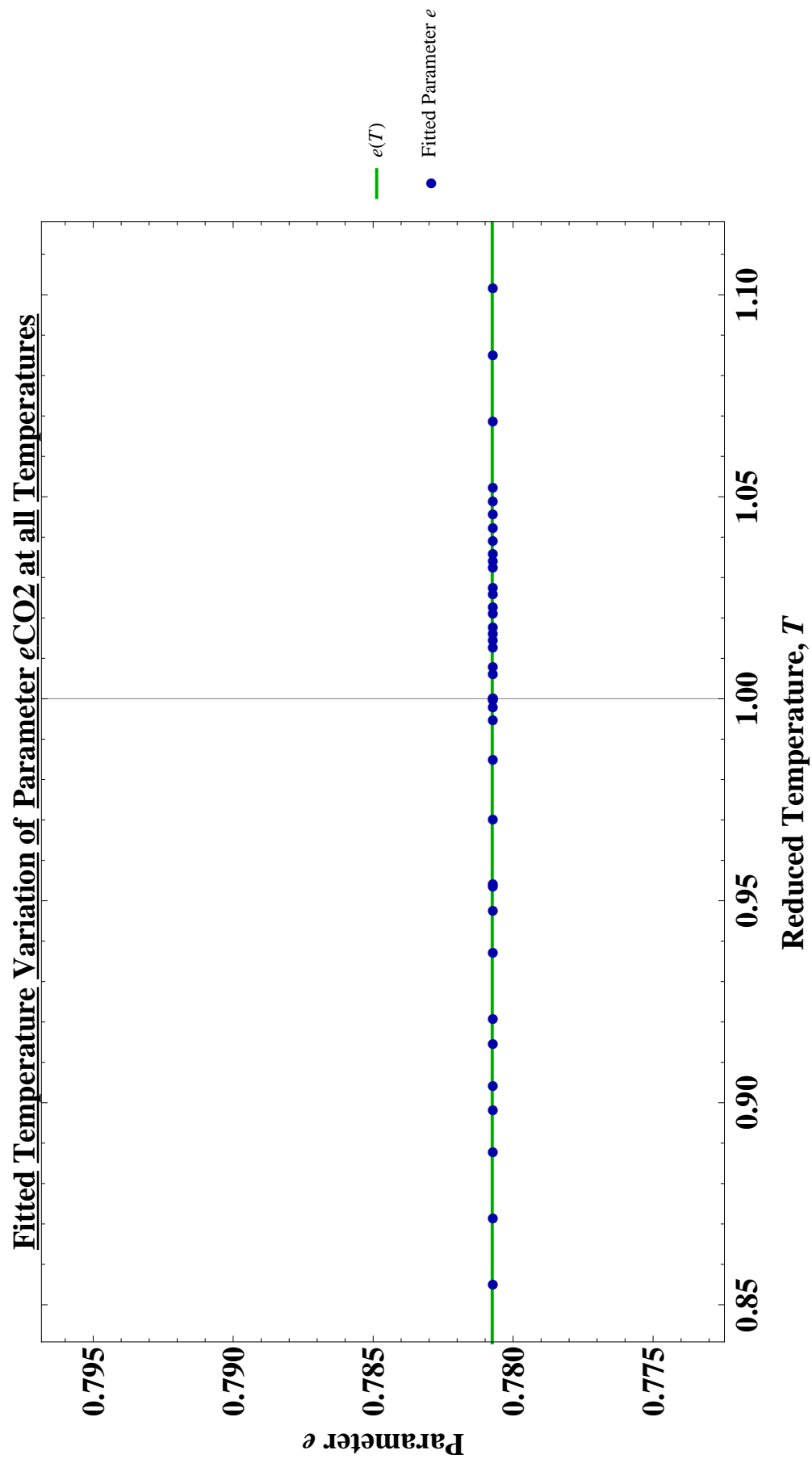


Figure 4.19: Variation of parameter e_{CO_2} at all temperatures in the CCS pipeline relevant range

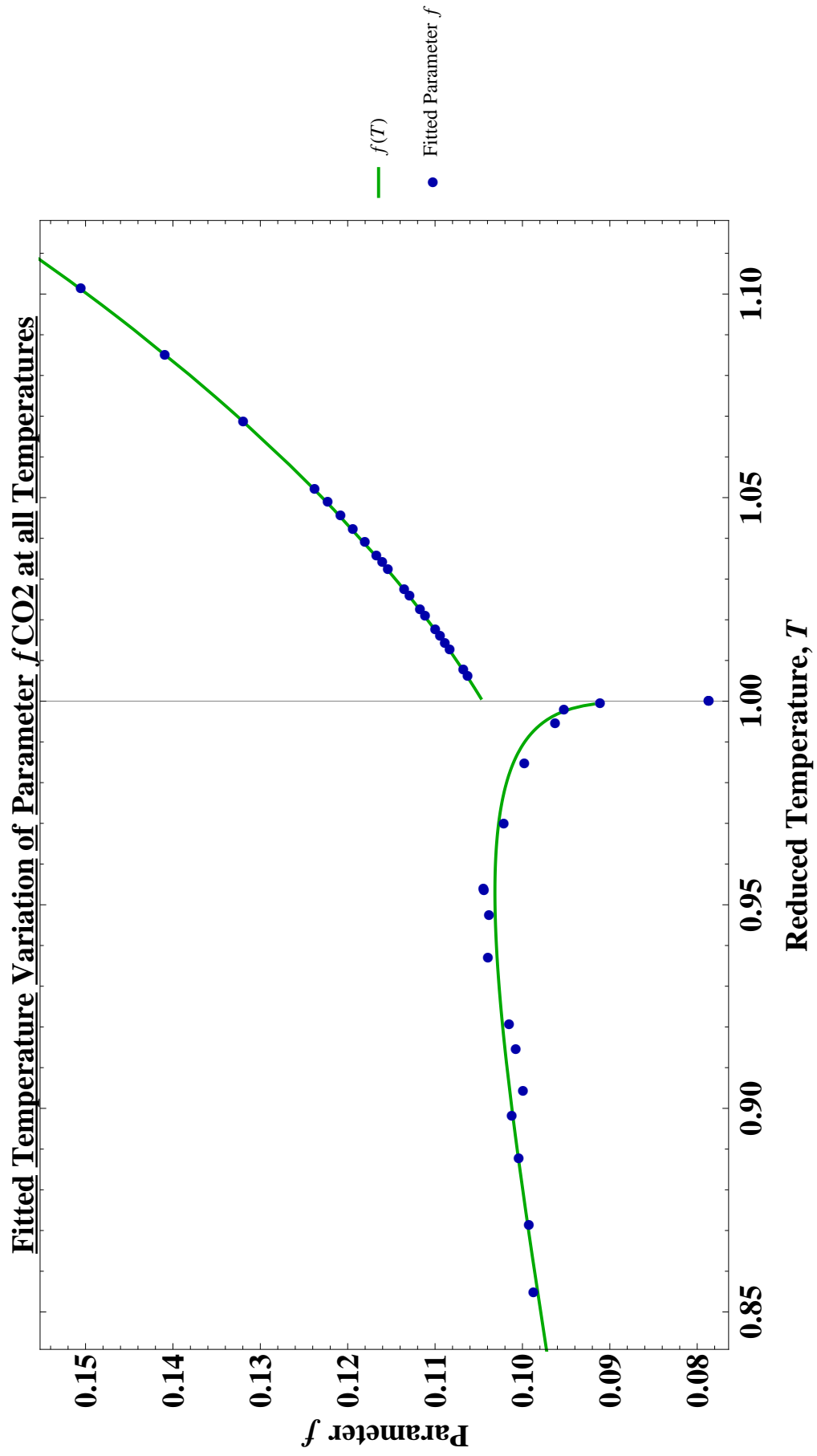


Figure 4.20: Variation of parameter f_{CO_2} at all temperatures in the CCS pipeline relevant range

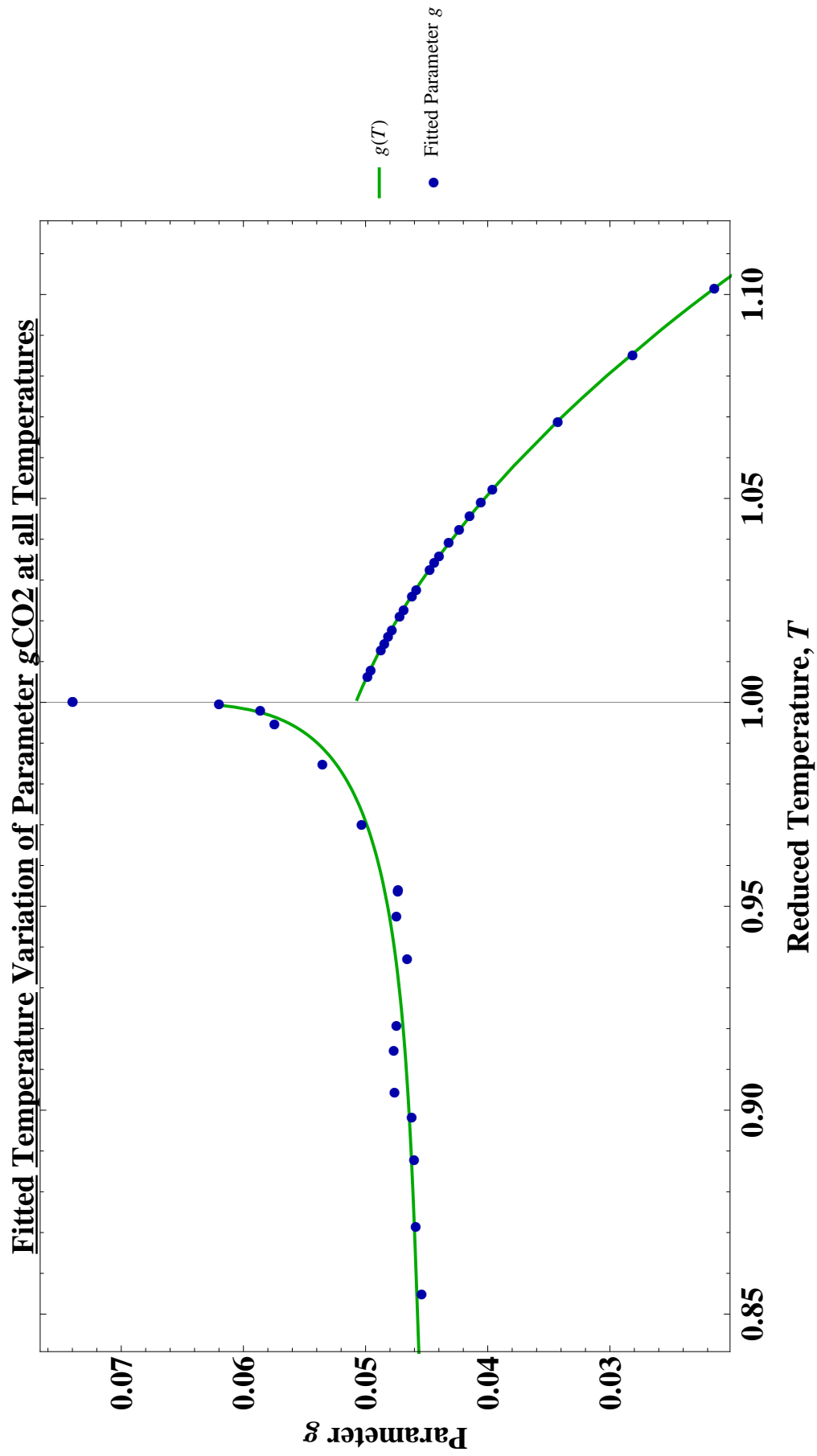


Figure 4.21: Variation of parameter g_{CO_2} at all temperatures in the CCS pipeline relevant range

Thus each parameter was fully defined and this completed the model in the case of pure carbon dioxide. We note that the parameter variations given here differ slightly from those proposed in our published work [40]. The model proposed here extends to the elevated temperatures, and has a better performance than that suggested previously.

4.5 Performance of the Proposed Model in the Case of Pure Carbon Dioxide

Having established the continuous temperature dependences for each model parameter, we subsequently found our model to very accurately reconstruct the data provided by NIST. Over the following pages we have plotted the behaviour at a range of different temperatures (including T_c) throughout the range of relevance for CCS pipelines in order to demonstrate the usefulness of the proposed equation within this range.

Figures 4.22 to 4.31 show a direct comparison between pressure predictions of our equation of state (dark green line) and the Peng–Robinson equation of state (dark red line) against the NIST data (dark blue markers), as well as the phase behaviour in the form of the bubble and dew points, shown for each model by triangles in its respective colour, and for the NIST data by the large hollow triangles. We can easily verify that the proposed model (3.21) incorporating parameters a to g as defined in Equations (4.7), (4.9), (4.10), (4.11), (4.12), (4.13) and (4.14) gives a very accurate description.

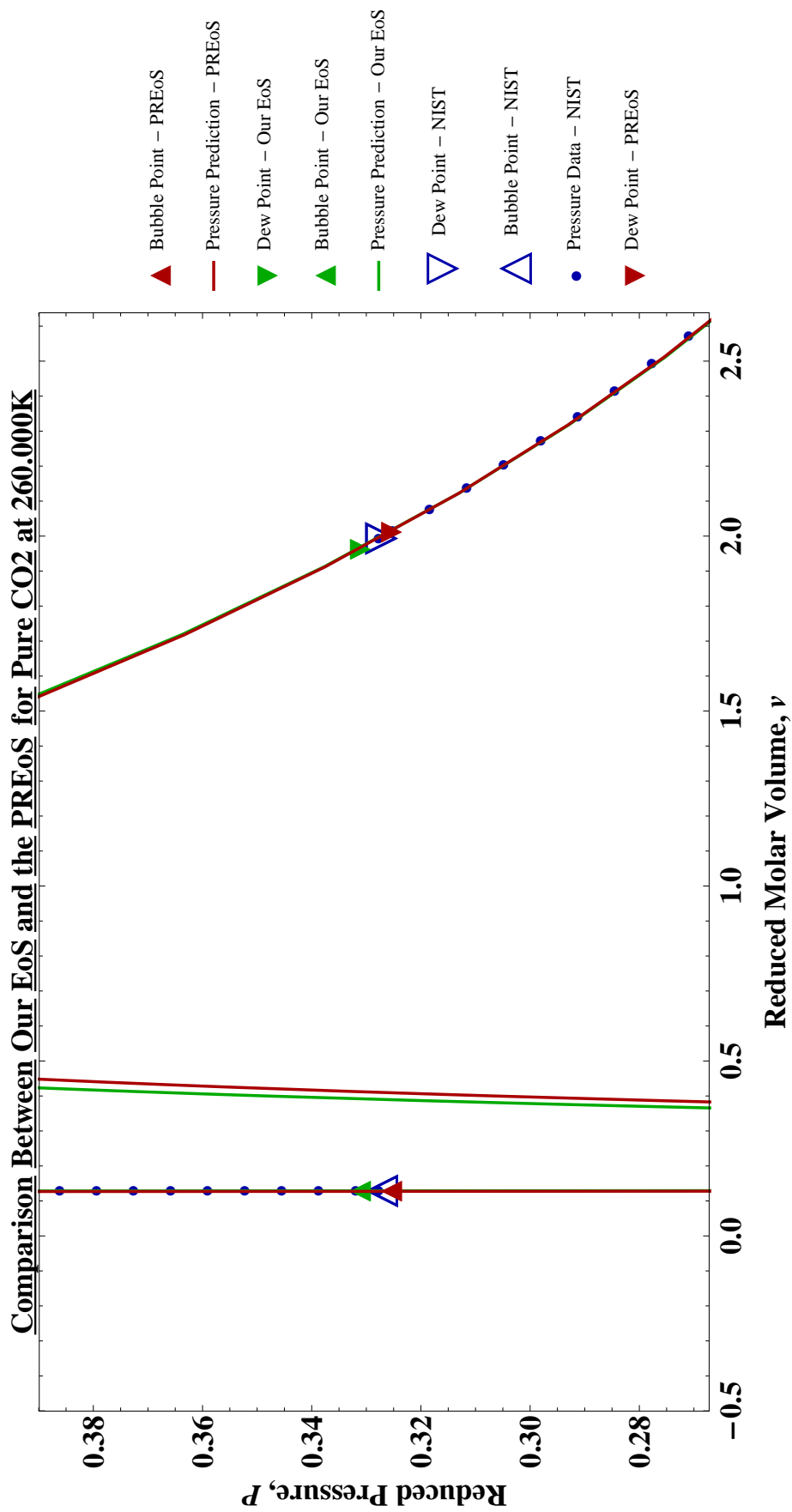


Figure 4.22: A comparison between the proposed EoS and the PREoS against the NIST data at 260K

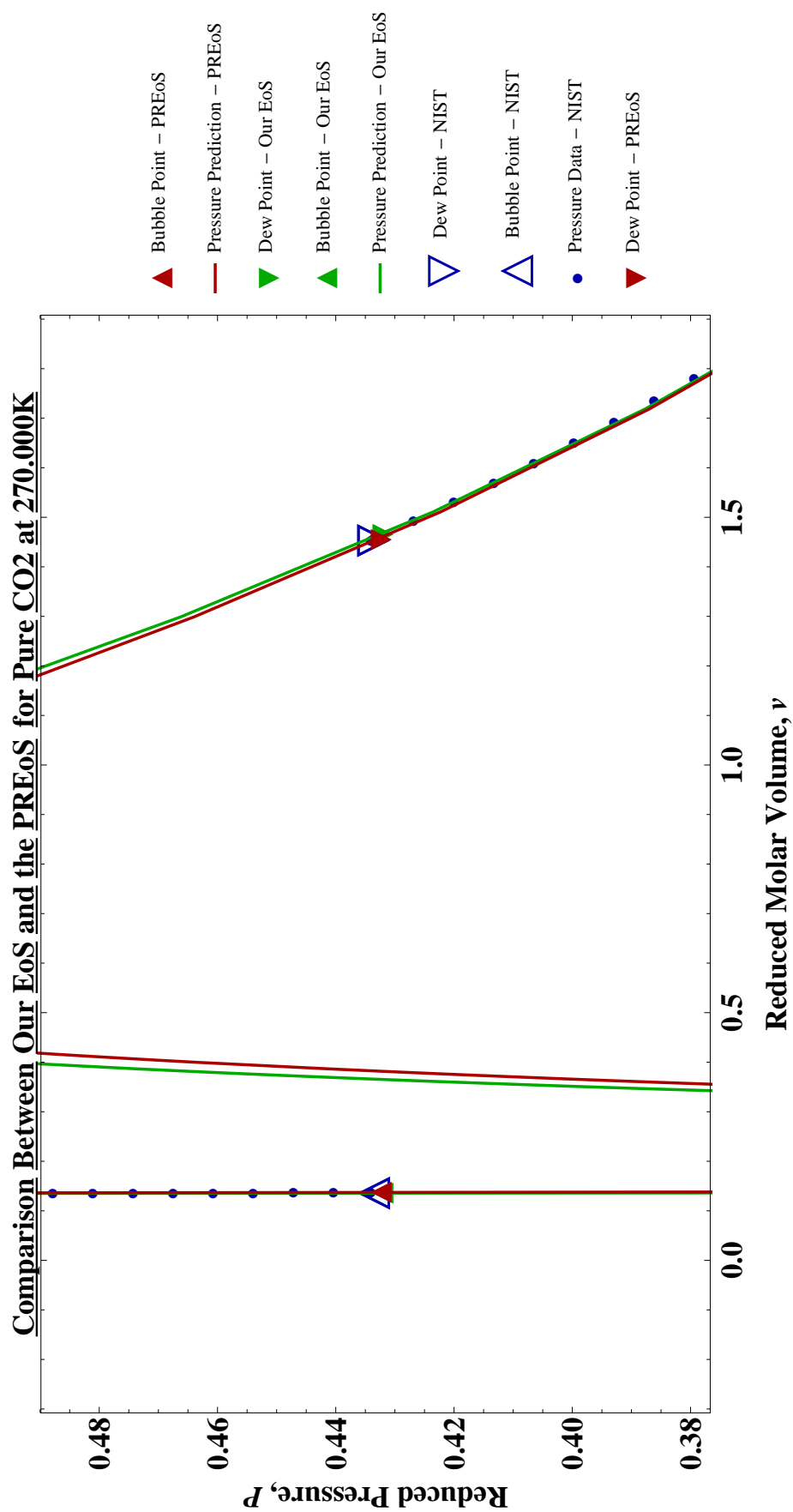


Figure 4.23: A comparison between the proposed EoS and the PREoS against the NIST data at 270K

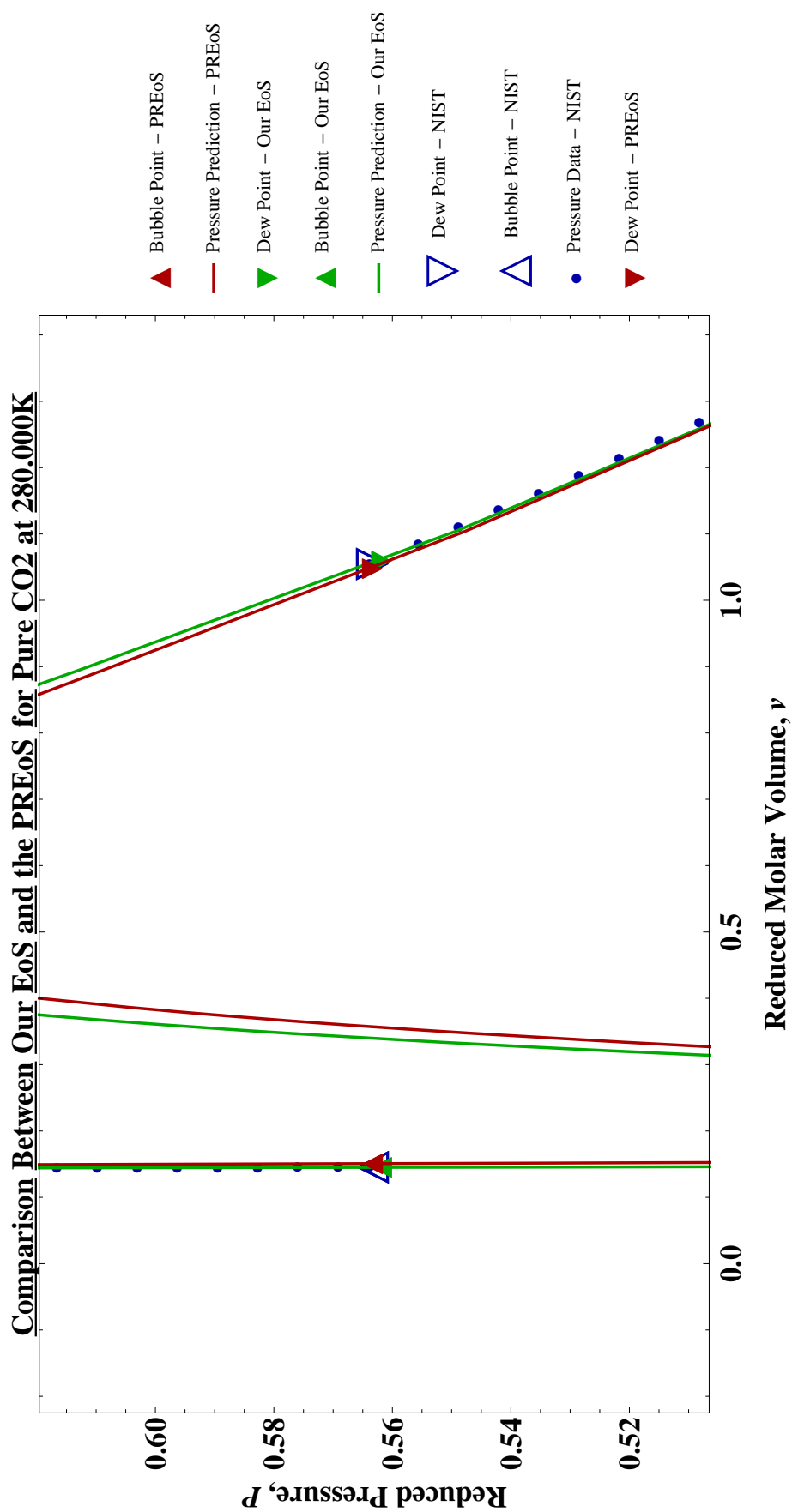


Figure 4.24: A comparison between the proposed EoS and the PREoS against the NIST data at 280K

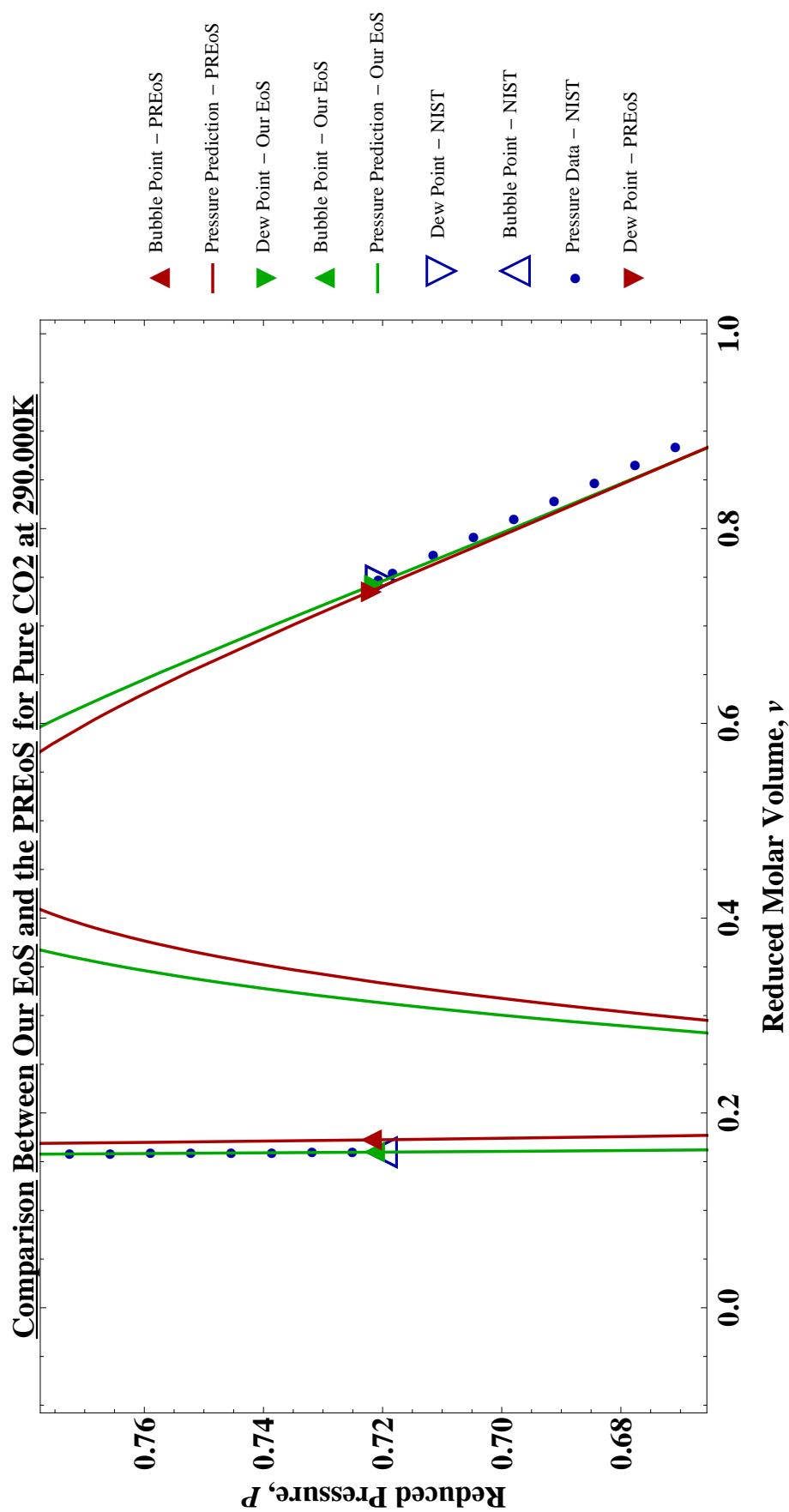


Figure 4.25: A comparison between the proposed EoS and the PREoS against the NIST data at 290K

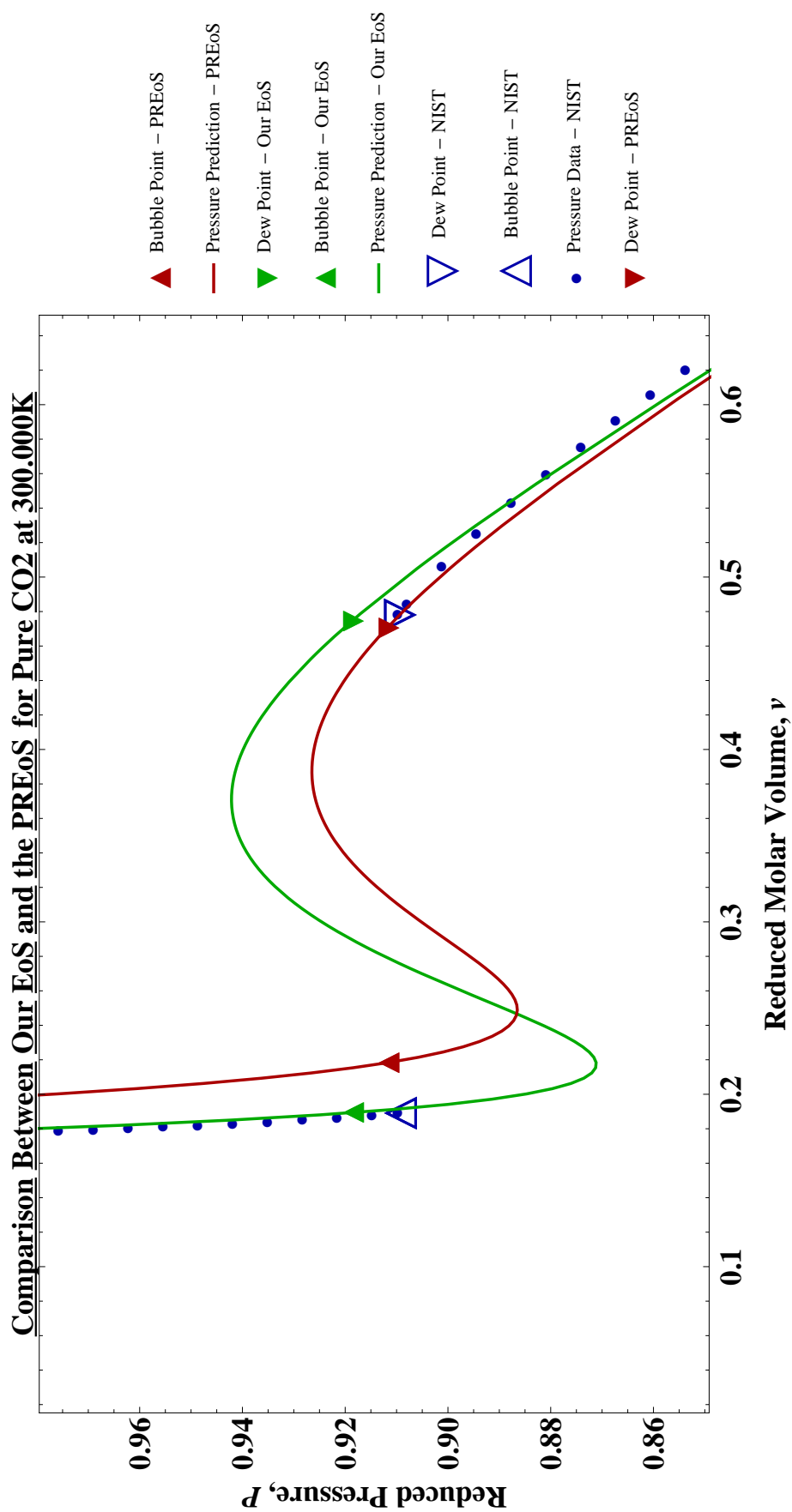


Figure 4.26: A comparison between the proposed EoS and the PREoS against the NIST data at 300K

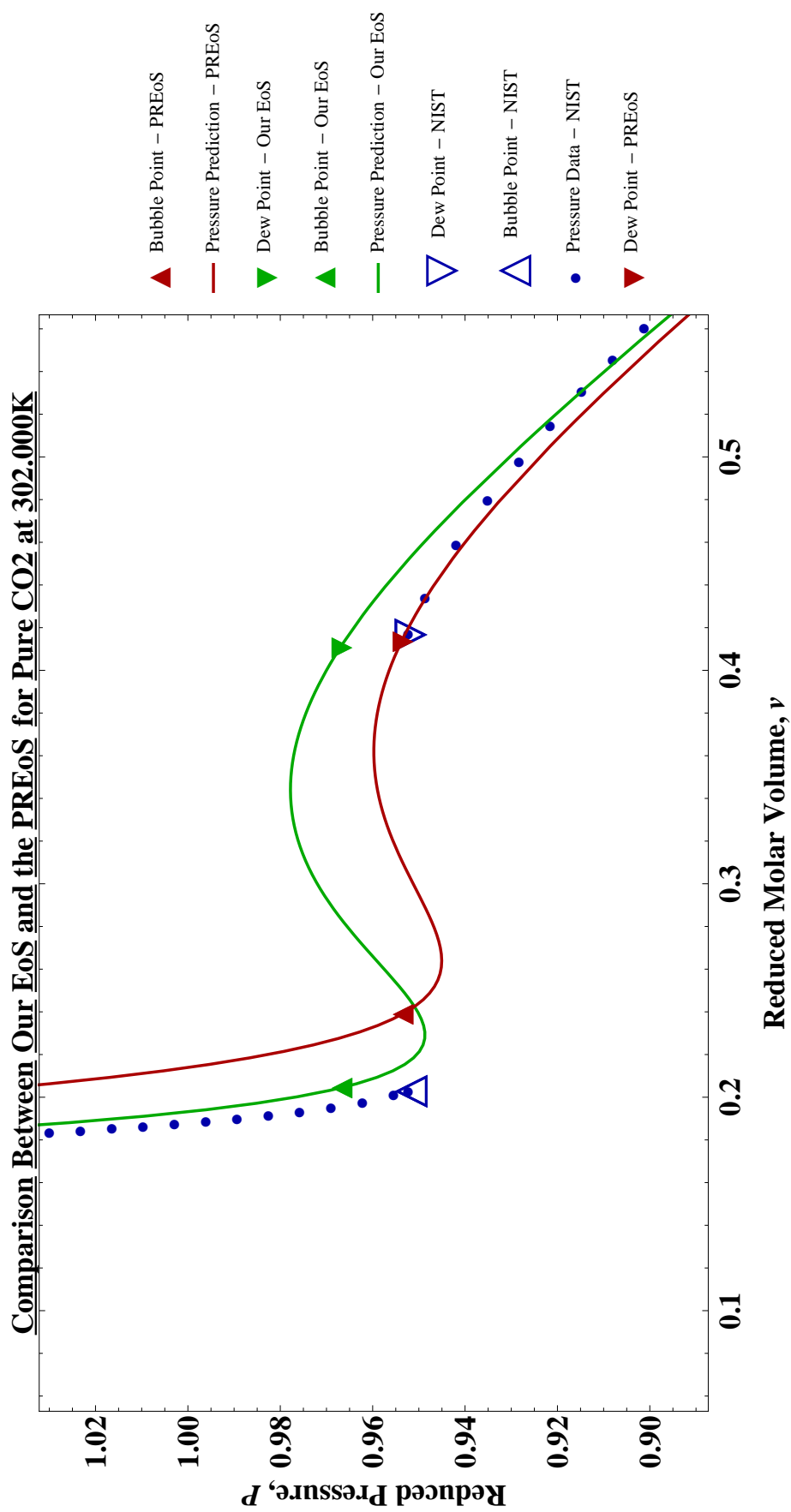


Figure 4.27: A comparison between the proposed EoS and the PREoS against the NIST data at 302K

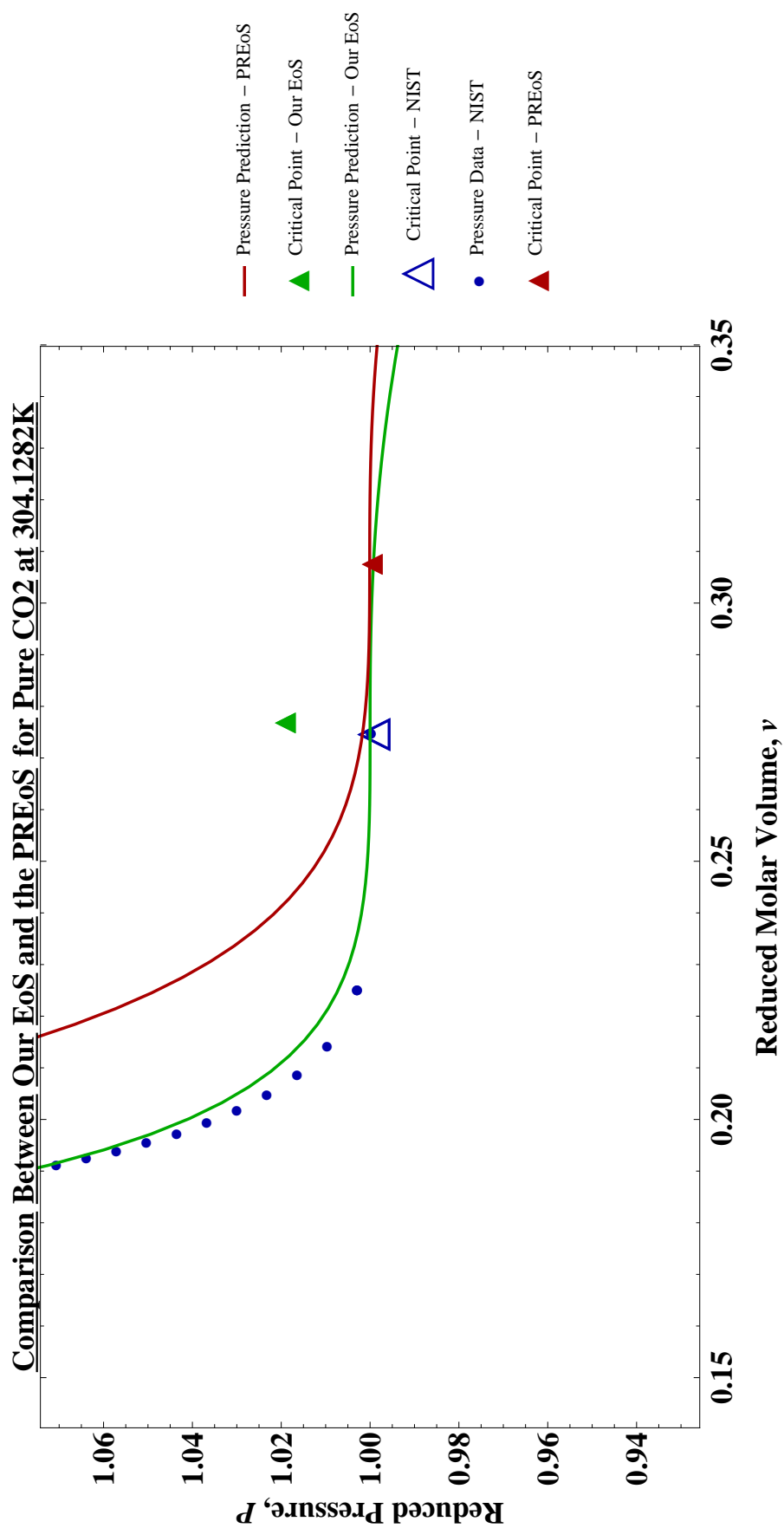


Figure 4.28: A comparison between the proposed EoS and the PREoS against the NIST data at the critical temperature

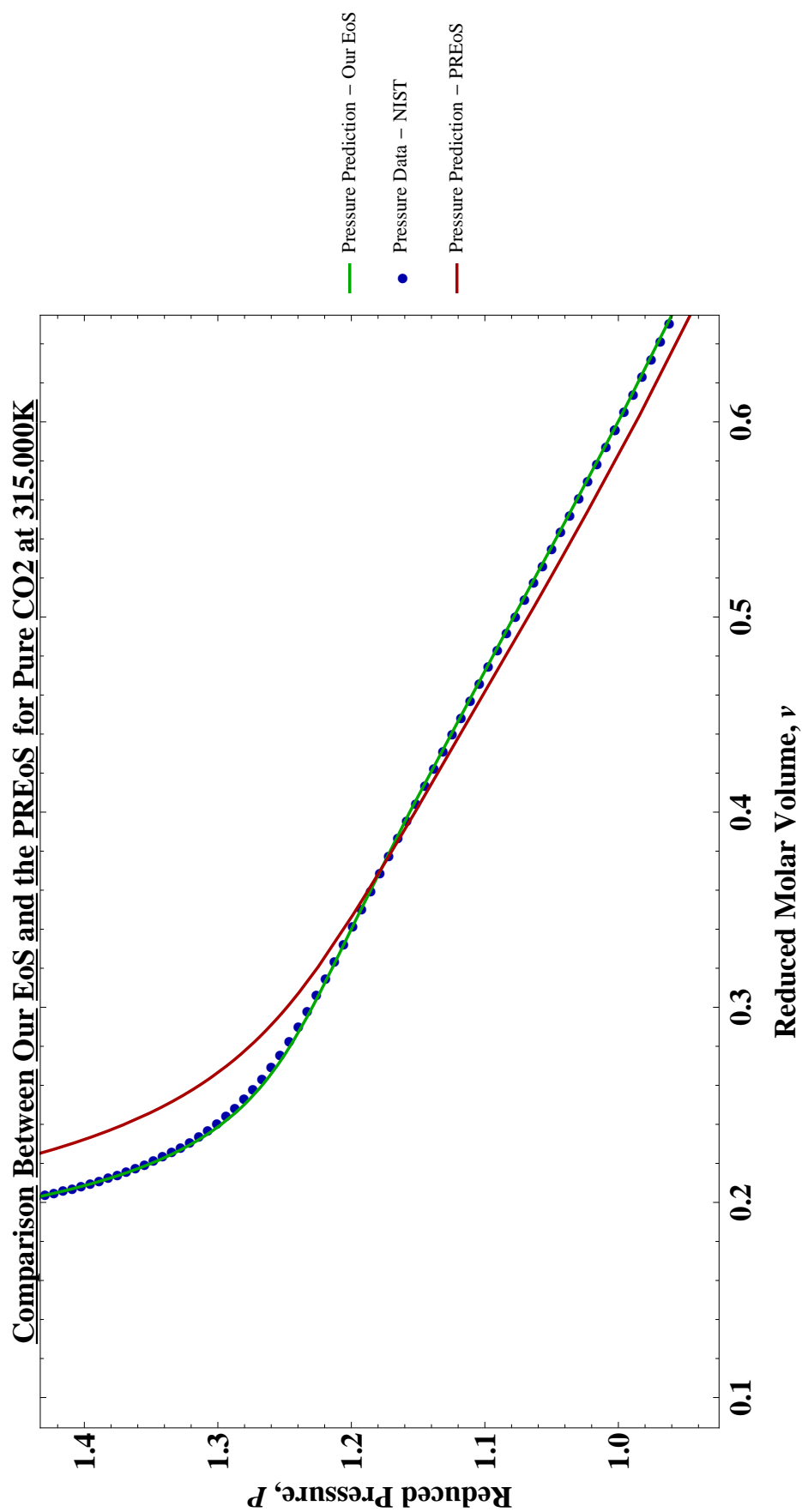


Figure 4.29: A comparison between the proposed EoS and the PREoS against the NIST data at 315K

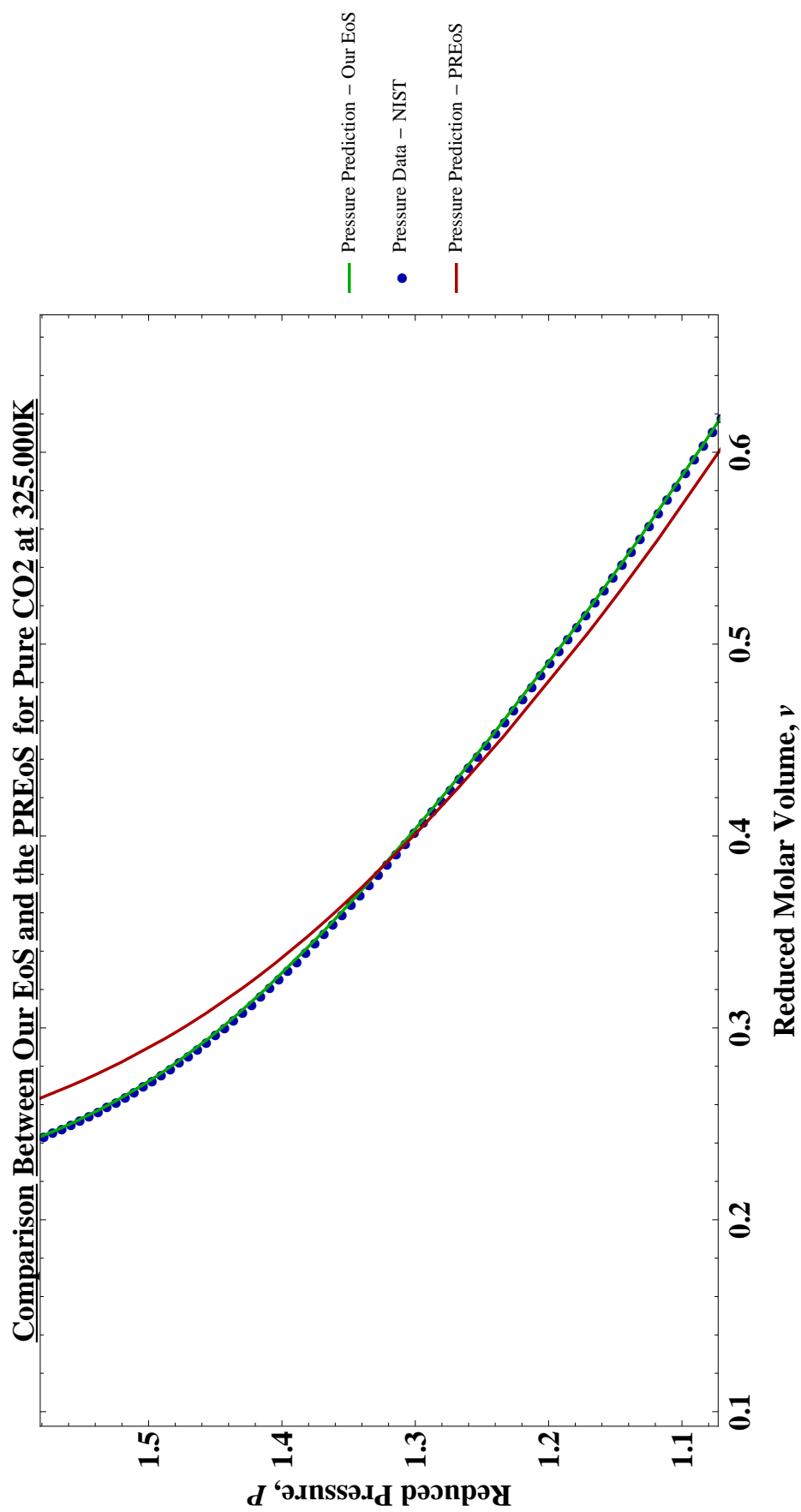


Figure 4.30: A comparison between the proposed EoS and the PREoS against the NIST data at 325K

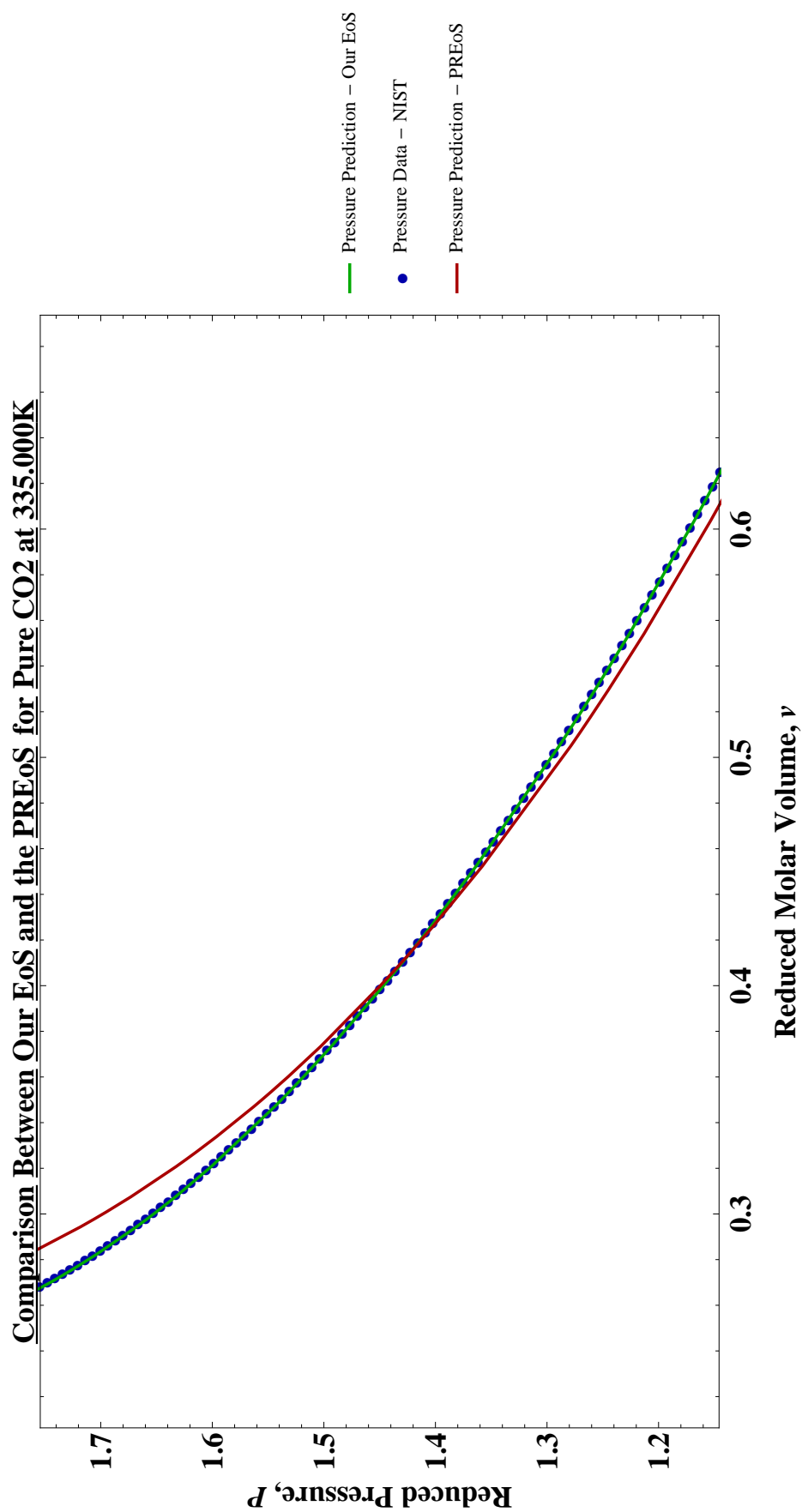


Figure 4.31: A comparison between the proposed EoS and the PREoS against the NIST data at 335K

In particular, we note the following:

- In the high pressure region there is a much better agreement with the NIST data for our model than PREoS.
- We also note the closeness of agreement with the NIST bubble and dew points and the predicted bubble and dew points of the proposed EoS, thus suggesting that our model is as accurate as had aimed for.
- Looking closely at the multi-phase region we can see that in the liquid phase, the PREoS fails to model the pressure behaviour accurately enough for CCS. In this region, we can see from Table 4.2 that it can be as much as 41% out in the relevant range of temperatures, whereas the proposed EoS never exhibits more than a 5.5% error compared to the NIST data, and rarely more than a 2% error.

Broadly speaking we found the proposed model to very accurately reconstruct the pressure and phase behaviour prescribed by the NIST database. The phase behaviour was generally found to be well within our target range of a 2% error, as shown in Table 4.2. Specifically, we found the pressure predictions to almost exclusively be within this target range, apart from in the immediate vicinity of the critical point. We conjecture that having enforced the model to vary smoothly, this may account for the slight loss of comparable accuracy in this region. Despite this however, we note that our model still appears to offer significant advantages in accuracy over the PREoS.

The values for percentage errors are given in the Table 4.2, with a comparison against the PREoS demonstrating the potential of our model. For the proposed equation, percentage errors were calculated using Equation (4.1), and for the PREoS an analogous equation was used. In Table 4.3 we also note the critical property predictions of the proposed model, and Figure 4.32 compares the prediction of the pure case phase boundary made by our model to that of the PREoS.

| Temperature (K) | Maximum Percentage Error in P | | Average Percentage Error in P | | Percentage Error in P_{vap} | | Percentage Error in v_{BP} | | Percentage Error in v_{DP} | |
|--------------------|---------------------------------------|--------|---------------------------------------|--------|-------------------------------------|-------|------------------------------------|--------|------------------------------------|-------|
| | (3.21) | PREoS | (3.21) | PREoS | (3.21) | PREoS | (3.21) | PREoS | (3.21) | PREoS |
| 260 | 14.979 | 45.332 | 1.730 | 38.109 | 1.068 | 0.664 | 0.113 | 0.991 | 1.520 | 0.847 |
| 265 | 2.672 | 38.337 | 1.746 | 25.379 | 0.004 | 0.520 | 0.052 | 0.013 | 0.099 | 0.528 |
| 270 | 4.093 | 31.811 | 2.467 | 17.202 | 0.439 | 0.365 | 0.038 | 1.053 | 0.793 | 0.161 |
| 273.15 | 4.259 | 31.564 | 2.291 | 14.320 | 0.500 | 0.265 | 0.233 | 1.624 | 0.886 | 0.093 |
| 275 | 3.848 | 35.412 | 2.052 | 13.029 | 0.484 | 0.207 | 0.060 | 2.264 | 0.845 | 0.248 |
| 278.15 | 2.734 | 39.602 | 1.560 | 11.472 | 0.400 | 0.109 | 0.090 | 3.088 | 0.651 | 0.524 |
| 280 | 2.002 | 40.852 | 1.264 | 10.765 | 0.329 | 0.053 | 0.087 | 3.627 | 0.481 | 0.691 |
| 285 | 1.363 | 40.529 | 0.670 | 9.463 | 0.106 | 0.084 | 0.105 | 5.236 | 0.091 | 1.147 |
| 288.15 | 1.551 | 38.005 | 0.564 | 8.944 | 0.035 | 0.157 | 0.019 | 6.555 | 0.449 | 1.425 |
| 290 | 1.654 | 35.814 | 0.582 | 8.627 | 0.117 | 0.191 | 0.048 | 7.375 | 0.625 | 1.574 |
| 290.15 | 1.662 | 35.615 | 0.584 | 8.639 | 0.123 | 0.194 | 0.041 | 7.436 | 0.638 | 1.586 |
| 291 | 1.705 | 34.431 | 0.599 | 8.533 | 0.161 | 0.207 | 0.150 | 7.929 | 0.702 | 1.649 |
| 292 | 1.752 | 32.913 | 0.618 | 8.364 | 0.208 | 0.221 | 0.148 | 8.413 | 0.764 | 1.717 |
| 293 | 1.793 | 31.267 | 0.639 | 8.207 | 0.257 | 0.232 | 0.059 | 8.846 | 0.808 | 1.776 |
| 293.15 | 1.798 | 31.009 | 0.643 | 8.218 | 0.264 | 0.234 | 0.090 | 8.953 | 0.813 | 1.784 |
| 294 | 1.827 | 29.531 | 0.663 | 8.132 | 0.311 | 0.240 | 0.076 | 9.404 | 0.834 | 1.825 |
| 294.5 | 1.842 | 28.715 | 0.675 | 8.024 | 0.340 | 0.243 | 0.128 | 9.735 | 0.839 | 1.844 |
| 295 | 1.854 | 27.945 | 0.688 | 7.989 | 0.372 | 0.245 | 0.041 | 9.950 | 0.838 | 1.859 |
| 295.5 | 1.864 | 27.218 | 0.701 | 7.888 | 0.407 | 0.246 | 0.007 | 10.207 | 0.834 | 1.870 |
| 296 | 1.871 | 26.527 | 0.714 | 7.854 | 0.444 | 0.247 | 0.015 | 10.510 | 0.824 | 1.875 |
| 296.5 | 1.875 | 25.874 | 0.728 | 7.819 | 0.485 | 0.246 | 0.023 | 10.862 | 0.811 | 1.874 |
| 297 | 1.877 | 25.254 | 0.740 | 7.726 | 0.531 | 0.244 | 0.111 | 11.267 | 0.796 | 1.867 |
| 297.5 | 1.875 | 24.663 | 0.752 | 7.692 | 0.582 | 0.240 | 0.091 | 11.585 | 0.778 | 1.851 |
| 298 | 1.870 | 24.102 | 0.762 | 7.604 | 0.639 | 0.236 | 0.137 | 11.969 | 0.760 | 1.825 |
| 298.15 | 1.868 | 23.939 | 0.765 | 7.610 | 0.658 | 0.234 | 0.133 | 12.070 | 0.756 | 1.815 |
| 298.5 | 1.861 | 23.568 | 0.772 | 7.570 | 0.704 | 0.230 | 0.099 | 12.286 | 0.746 | 1.788 |
| 299 | 1.848 | 23.057 | 0.780 | 7.488 | 0.777 | 0.223 | 0.152 | 12.688 | 0.739 | 1.737 |
| 299.5 | 1.830 | 22.568 | 0.788 | 7.453 | 0.860 | 0.214 | 0.157 | 13.049 | 0.744 | 1.668 |
| 300 | 1.815 | 22.103 | 0.795 | 7.376 | 0.955 | 0.203 | 0.140 | 13.390 | 0.770 | 1.578 |
| 300.5 | 2.020 | 21.656 | 0.806 | 7.339 | 1.065 | 0.191 | 0.291 | 13.865 | 0.830 | 1.460 |
| 301 | 2.263 | 21.229 | 0.823 | 7.267 | 1.191 | 0.176 | 0.356 | 14.241 | 0.943 | 1.305 |
| 301.5 | 2.553 | 20.818 | 0.857 | 7.228 | 1.336 | 0.159 | 0.566 | 14.694 | 1.141 | 1.100 |
| 302 | 2.898 | 20.424 | 0.924 | 7.162 | 1.506 | 0.139 | 0.757 | 15.038 | 1.481 | 0.819 |
| 302.5 | 3.307 | 20.044 | 1.081 | 7.099 | 1.702 | 0.116 | 1.313 | 15.507 | 2.078 | 0.421 |
| 303 | 3.792 | 19.680 | 1.319 | 7.057 | 1.925 | 0.090 | 2.321 | 15.936 | 3.214 | 0.182 |
| 303.15 | 3.952 | 19.573 | 1.403 | 7.034 | 1.996 | 0.081 | 2.822 | 16.063 | 3.765 | 0.429 |
| 303.5 | 4.343 | 19.329 | 1.630 | 7.000 | 2.157 | 0.058 | 4.815 | 16.329 | 5.952 | 1.217 |
| 304 | 4.628 | 18.990 | 1.963 | 6.945 | 2.137 | 0.020 | 11.017 | 16.015 | 16.092 | 3.849 |
| 304.1282 | 5.483 | 18.905 | 2.141 | 6.922 | — | — | — | — | — | — |
| 304.5 | 1.450 | 18.664 | 0.453 | 6.902 | — | — | — | — | — | — |
| 305 | 1.405 | 18.349 | 0.365 | 6.863 | — | — | — | — | — | — |
| 305.5 | 1.405 | 18.349 | 0.365 | 6.863 | — | — | — | — | — | — |
| 306 | 1.342 | 18.044 | 0.303 | 6.823 | — | — | — | — | — | — |
| 306.5 | 1.279 | 17.750 | 0.256 | 6.784 | — | — | — | — | — | — |
| 307 | 1.217 | 17.465 | 0.225 | 6.743 | — | — | — | — | — | — |
| 307.5 | 1.157 | 17.189 | 0.204 | 6.701 | — | — | — | — | — | — |
| 308 | 1.098 | 16.922 | 0.187 | 6.658 | — | — | — | — | — | — |
| 308.5 | 1.041 | 16.663 | 0.175 | 6.614 | — | — | — | — | — | — |
| 309 | 0.984 | 16.411 | 0.165 | 6.569 | — | — | — | — | — | — |
| 309.5 | 0.929 | 16.167 | 0.156 | 6.523 | — | — | — | — | — | — |
| 310 | 0.874 | 15.931 | 0.150 | 6.476 | — | — | — | — | — | — |
| 310.5 | 0.820 | 15.701 | 0.144 | 6.429 | — | — | — | — | — | — |
| 311 | 0.770 | 15.478 | 0.138 | 6.380 | — | — | — | — | — | — |
| 311.5 | 0.721 | 15.261 | 0.133 | 6.331 | — | — | — | — | — | — |
| 312 | 0.672 | 15.049 | 0.127 | 6.281 | — | — | — | — | — | — |
| 312.5 | 0.624 | 14.844 | 0.122 | 6.230 | — | — | — | — | — | — |
| 313 | 0.530 | 14.449 | 0.110 | 6.126 | — | — | — | — | — | — |
| 313.5 | 0.485 | 14.260 | 0.104 | 6.073 | — | — | — | — | — | — |
| 314 | 0.440 | 14.075 | 0.098 | 6.019 | — | — | — | — | — | — |
| 314.5 | 0.399 | 13.896 | 0.091 | 5.965 | — | — | — | — | — | — |
| 315 | 0.358 | 13.720 | 0.084 | 5.911 | — | — | — | — | — | — |
| 316 | 0.279 | 13.383 | 0.070 | 5.800 | — | — | — | — | — | — |
| 317 | 0.205 | 13.062 | 0.057 | 5.687 | — | — | — | — | — | — |
| 318 | 0.138 | 12.756 | 0.046 | 5.574 | — | — | — | — | — | — |
| 319 | 0.119 | 12.465 | 0.039 | 5.459 | — | — | — | — | — | — |
| 320 | 0.138 | 12.187 | 0.038 | 5.343 | — | — | — | — | — | — |
| 325 | 0.209 | 10.968 | 0.099 | 4.762 | — | — | — | — | — | — |
| 330 | 0.150 | 9.971 | 0.080 | 4.192 | — | — | — | — | — | — |
| 335 | 0.143 | 9.132 | 0.061 | 3.655 | — | — | — | — | — | — |

Table 4.2: Maximum and average percentage errors in P , and errors for P_{vap} , v_{BP} and v_{DP} for both the proposed EoS and the PREoS

| Model | Critical Temperature | | Critical Pressure | | Critical Volume | |
|----------------|----------------------|-----------|-------------------|-----------|--|-----------|
| | Predicted (K) | Error (%) | Predicted (MPa) | Error (%) | Predicted ($\text{m}^3 \cdot \text{mol}^{-1}$) | Error (%) |
| PREoS | 304.121 | 0.002 | 7.3768 | 0.007 | 1.0537×10^{-4} | 11.957 |
| Proposed Model | 304.422 | 0.097 | 7.5210 | 1.948 | 9.4875×10^{-5} | 0.803 |
| Actual Value | 304.1282 | — | 7.3773 | — | 9.41185×10^{-5} | — |

Table 4.3: Comparison of critical point predictions

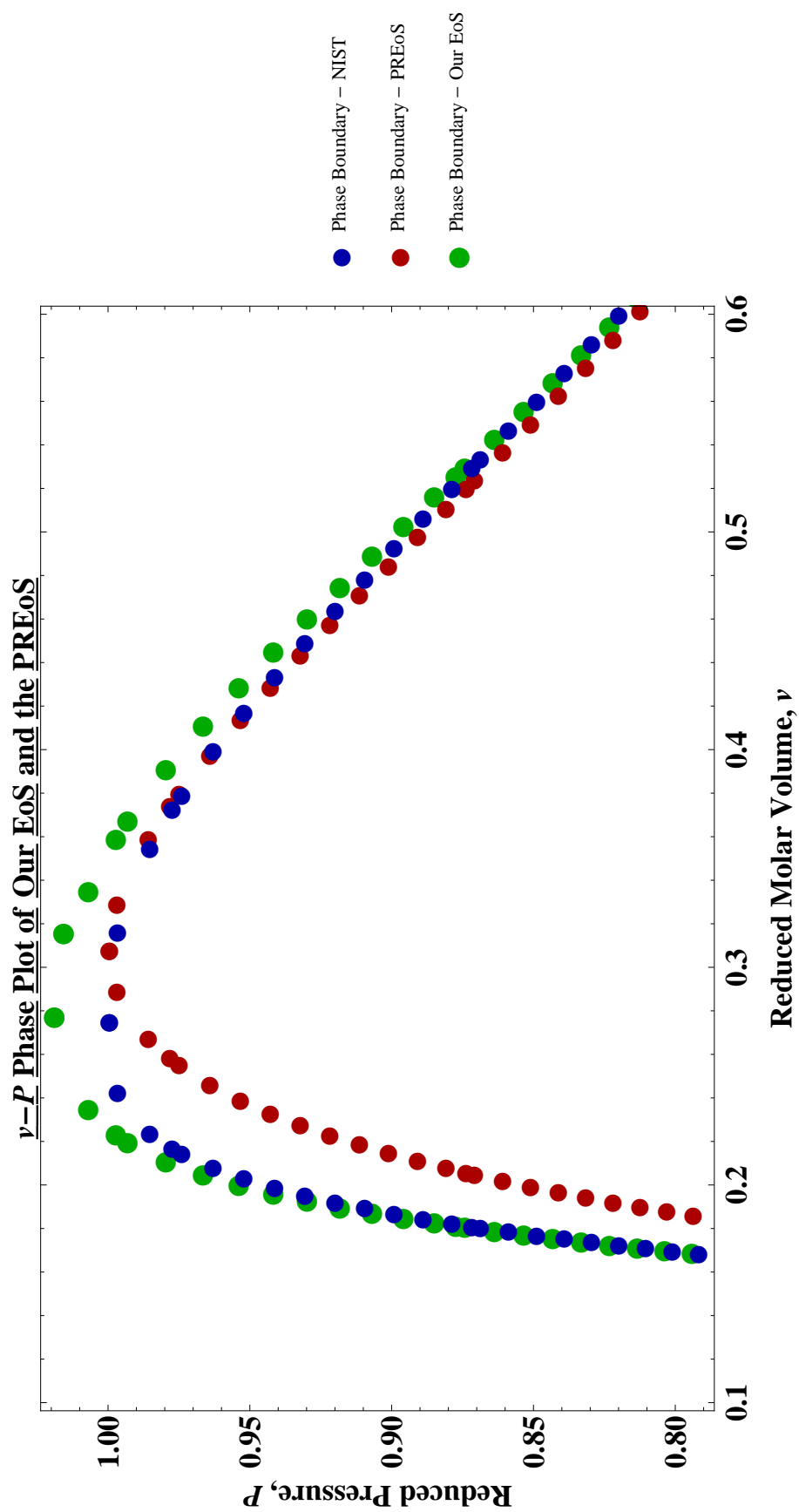


Figure 4.32: A comparison between predictions of the two-phase region boundary of our EoS compare to the PREoS

4.6 Discussion

As we can see from Figures 4.22 to 4.31 and 4.32, and Tables 4.2 and 4.3, the proposed equation of state certainly appears to have great potential in modelling the physical behaviour of pure carbon dioxide when compared directly with the PREoS, without any significant overburden of complexity. Our analyses revealed that there was hardly ever a time in the window 260–335K and 0.05–20MPa when the Peng–Robinson EoS predicted the pressure behaviour more accurately than the proposed EoS, except for when it happens to pass through zero error on the way from over–estimating to under–estimating (or vice–versa). The data in columns two to five of Table 4.2 substantiate this claim by showing that at any given temperature both the maximum and average errors of the proposed EoS compare extremely favourably to those of the Peng–Robinson EoS. This is definitely an excellent starting point from which to extend the EoS to a wider range of temperatures if deemed necessary and into predictions for physical behaviour of the CCS pipeline relevant mixtures.

Predictions of the bubble (v_{BP}, P_{vap}) and dew (v_{DP}, P_{vap}) points also seem to have been reasonably accurate although the proposed EoS is not quite so dominant over the Peng–Robinson EoS in this regard. In the region just below the critical point the Peng–Robinson EoS appears to do a better job of predicting the dew volume v_{DP} and the vapour pressure P_{vap} . We attribute this to our insistence that the model should give a smooth description of the behaviour at all temperatures, at the expense of some amount of the model’s flexibility, yielding an apparently unfavourable performance in this small region very close to the critical point. We also note the slight overestimation of the critical point, although with the intended application of this model to be the operation of CCS pipelines, this could ensure users err on the side of caution and stay away from the multi–phase region.

Nevertheless, we feel the model we proposed for the case of pure carbon dioxide is a significant step forward in modelling carbon dioxide behaviour in the CCS pipeline relevant region. We highlight that within the window of 260–335K and upto 200bar, our equation actually delivers its best performance in the region that really matters to CCS pipeline design and operation: the dense liquid and supercritical phases upto and including the liquid saturation line. The percentage errors we associate with our model were found, generally speaking, to be within our target range. At this stage of the research, we were happy to apply the pure CO₂ equation developed in this chapter to the case of binary mixtures.

Chapter 5

Calibration of the Binary Mixture Model

5.1 Generalising Fugacity Constraints to the Case of Mixtures

We begin this chapter by specifying a novel method which allows the fugacity of a substance when in mixture to be directly calculated from the fugacity when in the pure case. In Chapter 4, we established the pure fugacity constraint, which holds when a substance is on its own. The method we will show here allows us to enforce the fugacity requirements much more conveniently whilst fitting the binary mixture data, and furthermore, this works for any given form of equation of state and any mixing rules.

For this process we return briefly to working with dimensional units. Assuming we have an equation of state which explicitly gives the pressure P as a function of the molar volume v and some model parameters $\mathbf{a}(N_i) = (a_1(N_i), a_2(N_i), \dots, a_m(N_i))$, where N_i is the number of moles of substance i , and m is the number of components in the mixture, we may consider P to be in the form $P = f(v, \mathbf{a}(N_i))$. Recalling Equation (2.3.1) from [72], given in a slightly different form in this thesis in Equation (1.19):

$$\log(\phi(V)) = \frac{1}{RT} \int_{\hat{V}=\infty}^{\hat{V}=V} \left(\frac{1}{\hat{V}} - \left(\frac{\partial P}{\partial N} \right)_{T, \hat{V}, N_{j \neq i}} \right) d\hat{V} - \log(Z), \quad (5.1)$$

we apply the chain rule to the derivative in the integrand:

$$\frac{\partial P}{\partial N_i} = \frac{\partial P}{\partial v} \frac{\partial v}{\partial N_i} + \sum_j^m \frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i} \quad (5.2)$$

$$= -\frac{V}{N^2} \frac{\partial P}{\partial v} + \sum_j^m \frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i} \quad (5.3)$$

$$= -\frac{V}{N^2} \frac{\partial P}{\partial(V/N)} + \sum_j^m \frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i} \quad (5.4)$$

$$= -\frac{V}{N} \frac{\partial P}{\partial V} + \sum_j^m \frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i}, \quad (5.5)$$

where $a_j(N_i)$ denotes the j th parameter in $\mathbf{a}(N_i)$. Substituting this expression for $\frac{\partial P}{\partial N_i}$ back into (1.19) gives

$$\begin{aligned} \log(\bar{\phi}_i(V)) &= \frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N} \frac{\partial P}{\partial \hat{V}} - \sum_j^m \frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i} \right) d\hat{V} \\ &\quad - \log(Z) \end{aligned} \quad (5.6)$$

$$\begin{aligned} &= \left[\frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N} \frac{\partial P}{\partial \hat{V}} \right) d\hat{V} - \log(Z) \right] \\ &\quad - \left[\frac{1}{RT} \sum_j^m \int_{\infty}^V \left(\frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i} \right) d\hat{V} \right]. \end{aligned} \quad (5.7)$$

Considering the first square-bracketed term of Equation (5.7):

$$\begin{aligned} \frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N} \frac{\partial P}{\partial \hat{V}} \right) d\hat{V} - \log(Z) &= \frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} \right) d\hat{V} \\ &\quad + \frac{1}{RT} \int_{\infty}^V \left(\frac{\hat{V}}{N} \frac{\partial P}{\partial \hat{V}} \right) d\hat{V}, \end{aligned} \quad (5.8)$$

and we perform integration by parts on the second integral on the right hand side of Equation (5.8) to get:

$$\frac{1}{RT} \int_{\infty}^V \left(\frac{\hat{V}}{N} \frac{\partial P}{\partial \hat{V}} \right) d\hat{V} = \frac{1}{RT} \left[\frac{P\hat{V}}{N} \right]_{\infty}^V - \frac{1}{RT} \int_{\infty}^V \left(\frac{P(\hat{V})}{N} \right) d\hat{V} \quad (5.9)$$

$$= Z - 1 - \frac{1}{RT} \int_{\infty}^V \left(\frac{P(\hat{V})}{N} \right) d\hat{V}, \quad (5.10)$$

and upon substituting this back into Equation (5.8) we get

$$\begin{aligned} \frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N} \frac{\partial P}{\partial \hat{V}} \right) d\hat{V} - \log(Z) &= \frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} - \frac{P}{N} \right) d\hat{V} \\ &\quad - \log(Z) + Z - 1, \end{aligned} \quad (5.11)$$

the right hand side of which we recognise from Equation (2.3.9) in [72] as being the same expression for the fugacity coefficient in pure form, but with mixture parameters accounted for.

It would be beneficial if we could relate the two expressions for the pure and mixture case fugacity, as this would allow us to work out one from the other. We now considering the second square-bracketed term of (5.7), and begin by making the following definition:

$$F := \log(\phi_i(V)) + \log(Z) - Z + 1 \quad (5.12)$$

$$= \frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} - \frac{P}{N} \right) d\hat{V}, \quad (5.13)$$

where the second equality follows from Equation (2.8). We differentiate this expression for F with respect to a_j to get a term that can be used to simplify the second square-bracketed term in Equation (5.7):

$$N \frac{\partial F}{\partial a_j} = N \frac{\partial}{\partial a_j} \left(\frac{1}{RT} \int_{\infty}^V \left(\frac{RT}{\hat{V}} - \frac{P}{N} \right) d\hat{V} \right) \quad (5.14)$$

$$= \frac{1}{RT} \int_{\infty}^V \left(-N \frac{\partial}{\partial a_j} \left(\frac{P}{N} \right) d\hat{V} \right) \quad (5.15)$$

$$= \frac{1}{RT} \int_{\infty}^V \left(-\frac{\partial P}{\partial a_j} \right) d\hat{V}, \quad (5.16)$$

and substituting this into the second square bracket from Equation (5.7) gives

$$-\frac{1}{RT} \int_{\infty}^V \left(-\frac{\partial P}{\partial a_j} \frac{\partial a_j}{\partial N_i} \right) d\hat{V} = N \frac{\partial F}{\partial a_j} \frac{\partial a_j}{\partial N_i}. \quad (5.17)$$

Combining Equation (5.11) and (5.17) into Equation (5.7) gives

$$\log(\bar{\phi}_i(V)) = \log(\phi_i(V)) + N \sum_j^m \frac{\partial F}{\partial a_j} \frac{\partial a_j}{\partial N_i}. \quad (5.18)$$

Supposing then that we have model parameters \mathbf{a} (this vector notation meaning

(a, b, c, d, e, f, g) dependent on the relative molar concentrations of each chemical component in the mixture, such that for each parameter

$$a = a(\mathbf{x}), \quad (5.19)$$

where $\mathbf{x} = (x_1, x_2, \dots, x_n)$ is the vector of concentrations of chemical species within a mixture of n components. Now, since

$$\sum_i^n x_i = 1, \quad (5.20)$$

then by allowing the number of moles of each component to vary independently of the number of moles of other substances such that it is possible to increase the number of moles of one component without having to decrease another, we have:

$$x_i = \frac{N_i}{N_i + N_{\text{rest}}}, \quad (5.21)$$

$$x_j = \frac{N_j}{N_i + N_{\text{rest}}}, \quad (5.22)$$

where N_{rest} in this sense is the total number of moles of other substances. We can again apply the chain rule, this time to the second term of Equation (5.18), to obtain

$$\frac{\partial a_j}{\partial N_i} = \frac{\partial a_j}{\partial x_i} \frac{\partial x_i}{\partial N_i} + \sum_{k \neq i} \frac{\partial a_j}{\partial x_k} \frac{\partial x_k}{\partial N_i}. \quad (5.23)$$

Noting that

$$\frac{\partial x_i}{\partial N_i} = \frac{\partial}{\partial N_i} \left(\frac{N_i}{N_i + N_{\text{rest}}} \right) \quad (5.24)$$

$$= \frac{1}{N_i + N_{\text{rest}}} - \frac{N_i}{(N_i + N_{\text{rest}})^2} \quad (5.25)$$

$$= \frac{1}{N} - \frac{N_i}{N^2}, \quad (5.26)$$

$$(5.27)$$

in which case

$$N \frac{\partial x_i}{\partial N_i} = 1 - x_i, \quad (5.28)$$

and also that for $k \neq i$

$$\frac{\partial x_k}{\partial N_i} = \frac{\partial}{\partial N_i} \left(\frac{N_k}{N_i + N_{\text{rest}}} \right) \quad (5.29)$$

$$= -\frac{N_k}{(N_i + N_{\text{rest}})^2} \quad (5.30)$$

$$= -\frac{N_k}{N^2}, \quad (5.31)$$

$$(5.32)$$

whereby

$$N \frac{\partial x_k}{\partial N_i} = -x_k \quad (5.33)$$

for $k \neq i$. We can compile the effect of the mixing rules into Equation (5.18) to obtain a practical relation between the pure and mixture fugacity for chemical component i :

$$\log(\bar{\phi}_i(v)) = \log(\phi_i(v)) + \sum_j^m \frac{\partial F}{\partial a_j} \left(\frac{\partial a_j}{\partial x_i} - \sum_k^n x_k \frac{\partial a_j}{\partial x_k} \right). \quad (5.34)$$

We highlight Equation (5.34) as allowing us to conveniently evaluate the mixture fugacity constraint for component i , denoted $\log(\bar{\phi}_i(v))$, directly from the its pure fugacity constraint, denoted $\log(\phi_i(v))$, and the mixing rules $a_1(x_1, \dots, x_n)$, ..., $a_m(x_1, \dots, x_n)$.

5.2 Mixing Rules

As a chemical impurity is introduced to the mixture, we wish for our model to be able to predict the changes in pressure and phase behaviour that will be brought about as a result. In order to do this, we allow the model parameters to not merely vary with changing temperature, but also with the composition of the mixture. In this way, the effect of impurities can be included in the modelling of the CCS pipeline transport conditions.

Thus, for each parameter of the model we needed to propose a mixing rule. Returning now to dimensionless units, and taking inspiration from the mixing rules offered in the PREoS [34], we opted to impose the quadratic binary mixing rule for each of the model parameters in Equation (3.21) for increased flexibility. In the case of the

binary mixture for carbon dioxide and nitrogen for example, these are:

$$a(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 a_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} a_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 a_{\text{N}_2}(T) \quad (5.35)$$

$$b(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 b_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} b_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 b_{\text{N}_2}(T) \quad (5.36)$$

$$c(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 c_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} c_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 c_{\text{N}_2}(T) \quad (5.37)$$

$$d(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 d_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} d_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 d_{\text{N}_2}(T) \quad (5.38)$$

$$e(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 e_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} e_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 e_{\text{N}_2}(T) \quad (5.39)$$

$$f(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 f_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} f_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 f_{\text{N}_2}(T) \quad (5.40)$$

$$g(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}^2 g_{\text{CO}_2}(T) + x_{\text{CO}_2} x_{\text{N}_2} g_{\text{CO}_2, \text{N}_2}(T) + x_{\text{N}_2}^2 g_{\text{N}_2}(T), \quad (5.41)$$

where $a_{\text{CO}_2}(T)$, $b_{\text{CO}_2}(T)$, \dots are as defined in Chapter 4 for the pure carbon dioxide equation, $a_{\text{N}_2}(T)$, $b_{\text{N}_2}(T)$, \dots are the analogous quantities for nitrogen which we need to specify, and $a_{\text{CO}_2, \text{N}_2}(T)$, $b_{\text{CO}_2, \text{N}_2}(T)$, \dots are the binary interaction parameters, which also need to be determined.

We note at this stage that since in a binary system

$$x_{\text{N}_2} = 1 - x_{\text{CO}_2}, \quad (5.42)$$

the number of dependent variables for the mixing rules can be reduced to two. The above equations can be defined analogously for the other binary mixtures we are considering.

5.3 Carbon Dioxide–Nitrogen Binary Mixture

5.3.1 Data Availability

We begin this section by noting the literature data that was available for us to fit to for the CO_2 – N_2 mixture. As specified in Chapter 2, we would require isothermal VLE data including coexisting vapour and liquid points to be given at the same temperature as homogeneous phase density data. A tabulated summary of the relevant available data is given in Table 5.1, ordered by temperature.

We can see from Table 5.1 that the literature data contained just four temperature points where complete VLE data existed: at 273.15K [53, 54], 288.15K [53], 301.3K [91] and 303.3K [91], however, of these, we had to neglect the data at 303.3K on the grounds that it did not appear to give a true description of behaviour. We can also see from Table 5.1 that there were very few temperatures at which both VLE,

whether with volumes or not, and homogeneous density data existed. Without the estimation techniques described in Chapter 2, this would have left us with just two temperature points to fit the parameters for this particular binary system; 273.15K and 288.15K. With these methods, we were able to build the model around more temperature points.

| Temperature (K) | Homogeneous Density Data Sources | VLE Data Sources |
|-----------------|---|---|
| 260 | [82], [75], [88] | |
| 265 | [86], [83] | |
| 270 | [75], [88] | [95] [†] , [96] [†] , [97] [†] , [98] [†] |
| 273.15 | [53], [82], [99] | [53], [100] [†] , [54], [101] [†] , [102] [†] , [84] [†] , [103] [†] |
| 273.2 | | [104] [†] |
| 275 | [86], [83], [75], [88], [105] | |
| 280 | [75], [88] | |
| 285 | [86], [77], [83], [75], [88] | |
| 288.15 | [53] | [53], [100] [†] |
| 288.3 | | [106] [†] |
| 288.706 | [82] | |
| 290 | [75], [88] | |
| 293.2 | [107] | |
| 293.3 | | [106] [†] |
| 295 | [75], [88] | |
| 298.15 | [108] | [100] [†] |
| 298.2 | | [104] [†] |
| 300 | [82], [85], [86], [77], [83], [75], [88], [78], [105] | |
| 301.3 | | [91] |
| 303.22 | [109] | |
| 303.3 | | [91] |

[†] means the VLE data in this source did not contain volumes

Table 5.1: A summary of available data by source for carbon dioxide–nitrogen mixtures

5.3.2 Fitting the Carbon Dioxide–Nitrogen Binary Model Parameters

We proceeded first by determining the pure nitrogen parameters a_{N_2} to g_{N_2} at the available temperature points by the same sequence of optimisation techniques as used in the pure carbon dioxide case. Specifically, we minimised an error function which was exactly analogous to that in Equation (4.1), which in the case of a binary mixture, was

$$\begin{aligned}
E(a, b, c, d, e, f, g, h) = & W \sum_{i=1}^n \left(\frac{P(v_{\text{DATA}}^{(i)}, T, x_{\text{DATA}}^{(i)}) - P_{\text{DATA}}^{(i)}}{P_{\text{DATA}}^{(i)}} \right)^2 \\
& + (1 - W) \sum_{j=1}^m \left((\log \bar{\phi}_{\text{CO}_2}(v_{\text{DP}}^{(j)}) - \log \bar{\phi}_{\text{CO}_2}(v_{\text{BP}}^{(j)}))^2 \right. \\
& + (\log \bar{\phi}_{\text{N}_2}(v_{\text{DP}}^{(j)}) - \log \bar{\phi}_{\text{N}_2}(v_{\text{BP}}^{(j)}))^2 \\
& + (P(v_{\text{DP}}^{(j)}, T, x^{(j)}) - P_{\text{vap}}^{(j)})^2 \\
& \left. + (P(v_{\text{BP}}^{(j)}, T, x^{(j)}) - P_{\text{vap}}^{(j)})^2 \right), \tag{5.43}
\end{aligned}$$

where the first term after the equals sign is for fitting the homogeneous phase den-

sity and all subsequent terms are for fitting VLE at the phase boundary. In this equation n is the number of homogeneous density points at this temperature and m is the number of VLE coexistence points. Just as in the pure case, we minimised this initially by using simulated annealing at the first temperature point, then worked down the temperature values, at each subsequent one using local root finding.

In order to find the pure nitrogen parameter values, we temporarily introduced a linear mixing rule for each of the seven parameters, of the form

$$a_{\text{N}_2}(T, x_{\text{CO}_2}, x_{\text{N}_2}) = x_{\text{CO}_2}a_{\text{CO}_2}(T) + x_{\text{N}_2}a_{\text{N}_2}(T), \quad (5.44)$$

and similarly for parameters b_{N_2} through g_{N_2} . We did this because we found simulated annealing to struggle with more than seven parameters at any one time. In particular, we felt asking it to optimise an error function which was dependent on fourteen parameters would have been too demanding, and would have diminished the accuracy of the results it gave. We highlight that we were able to temporarily introduce this linear mixing rule as both it and the quadratic mixing rule as specified in Equation (5.35) give the same values when evaluated at either extreme of compositions.

Setting $W = 0.99$ to focus on fitting the homogeneous density data to begin with, we were able to generate values for each of the seven pure nitrogen parameters at each of the temperature points in this way. Having done this, we then reintroduced the quadratic mixing rules as given in Equation (5.35), in which both the pure carbon dioxide parameters a_{CO_2} and the pure nitrogen parameters a_{N_2} were now known. Following exactly the same procedure as having temporarily introduced a linear mixing rule, and setting $W = 0.05$ to allow the binary interaction parameters to focus on fitting the VLE behaviour, we repeated the process for the seven Binary Interaction Parameters (BIP) at each of the temperature points.

For the pure nitrogen parameters and the binary interaction parameters, the values we found by following this method are summarised in Table 5.2:

5.3.3 Preliminary Indications of Performance

After having found the fourteen parameters at each temperature point, we evaluated the performance of the proposed model to check the fitting that had been achieved through the optimisation of the error function (5.43) rendered a suitable representation of the data that had been used to calibrate it in each case.

| $T(K)$ | a_{N_2} | b_{N_2} | c_{N_2} | d_{N_2} | e_{N_2} | f_{N_2} | g_{N_2} |
|--------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 301.3 | -0.067690 | -0.069072 | 0.051949 | 0.394802 | 0.213906 | 0.707765 | -0.395181 |
| 298.15 | -0.112859 | -0.778754 | -1.142430 | 0.363730 | -0.088425 | 0.544037 | -0.269156 |
| 293.3 | 0.043030 | -0.306196 | -0.125938 | -0.225702 | -0.112868 | 0.996458 | -0.659658 |
| 288.15 | 0.021057 | -0.183572 | 0.028688 | -0.175184 | -0.126123 | 0.584742 | -0.321931 |
| 273.15 | 0.053949 | -0.146277 | 0.520106 | -0.192693 | -0.117818 | 0.631785 | -0.410574 |
| 270 | 0.009311 | -0.241595 | 0.451289 | -0.151992 | -0.126193 | 0.454463 | -0.243880 |

| $T(K)$ | a_{CO_2,N_2} | b_{CO_2,N_2} | c_{CO_2,N_2} | d_{CO_2,N_2} | e_{CO_2,N_2} | f_{CO_2,N_2} | g_{CO_2,N_2} |
|--------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 301.3 | 2.311730 | -1.546690 | -1.291800 | -3.533050 | -0.560407 | 1.616910 | -0.987250 |
| 298.15 | 0.422929 | -0.048641 | 0.067566 | -1.071050 | -0.655508 | 0.409527 | -0.071220 |
| 293.3 | 1.392655 | -0.491103 | 0.706931 | -1.985994 | 1.171984 | -0.036535 | 0.177126 |
| 288.15 | 0.128213 | 0.410874 | 0.907126 | 0.527336 | -2.189245 | 0.330155 | -0.040261 |
| 273.15 | 0.112001 | 0.639749 | 0.926503 | 0.296718 | -1.149070 | 0.450452 | -0.150223 |
| 270 | 2.872352 | 2.739344 | 3.937239 | -1.362795 | -1.182876 | -0.290171 | -0.124155 |

Table 5.2: Fitted parameter values for the carbon dioxide–nitrogen binary system

We did this by checking the percentage errors of the values suggested by our model for both the homogeneous density and VLE. A summary is in Table 5.3.

| Temperature (K) | Homogeneous Density | | v_{BP} † | | v_{DP} † | | x_{N_2} † | | y_{N_2} † | |
|--------------------|---------------------|---------|------------|---------|------------|---------|-------------|---------|-------------|---------|
| | Maximum | Average | Maximum | Average | Maximum | Average | Maximum | Average | Maximum | Average |
| 301.3 | 34.23 | 4.45 | 15.34 | 11.84 | 31.35 | 23.92 | 1.40 | 1.05 | 3.09 | 1.78 |
| 298.15 | 19.77 | 6.70 | 17.14 | 17.14 | 94.13 | 94.13 | 3.84 | 3.84 | 14.17 | 14.17 |
| 293.3 | 18.80 | 6.21 | 7.52 | 3.31 | 33.00 | 11.96 | 2.50 | 1.13 | 8.19 | 2.41 |
| 288.15 | 9.56 | 2.97 | 21.75 | 10.61 | 32.36 | 14.12 | 5.92 | 4.02 | 21.17 | 8.15 |
| 273.15 | 9.20 | 1.79 | 13.26 | 5.78 | 40.64 | 19.64 | 12.74 | 5.37 | 36.98 | 21.70 |
| 270 | 135.14 | 43.56 | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |

† where convergence to a meaningful solution had been possible

Table 5.3: Preliminary testing of predictions made by our model for the carbon dioxide–nitrogen binary system

We note at this stage that there was a particularly good fit of all the data types at 293.3K, 288.15K, and 273.15K. At these temperatures, where a relevant fitting had been achieved, a good behaviour was allowed by our proposed model and fitting technique. With the exception of the temperature points at which a poor fit had been achieved (301.3K, 298.15K, 270K), the average percentage errors for all quantities fell close to or under our target of 5%. We highlight in particular a very good fit to the homogeneous density data at the other three temperature points (293.3K, 288.15K, 273.15K). Unsurprisingly, when a poor fit had been found, the errors were quite large, and at 270K where a very poor fit had been found, convergence of the numerical search algorithms in finding the VLE had not been possible at all. With performance at 293.3K, 288.15K, and 273.15K having been demonstrated as being very reasonable, we fit the temperature dependence of the fourteen mixture parameters to the values taken at these points, discarding the parameter values at the other temperature points.

5.3.4 Variation of Model Parameters with Temperature

For each parameter we thus had only three temperature values at which reliable behaviour had been demonstrated. Analysing the values of the parameters at these three temperatures, we decided to fit a quadratic dependence, such as

$$a_{\text{N}_2}(T) = \alpha_1 T^2 + \alpha_2 T + \alpha_3, \quad (5.45)$$

where α_1 , α_2 , and α_3 would allow us to fit the values given in Table 5.2, and analogously for the other thirteen parameters.

In order to find the numerical values for α_1 , α_2 , and α_3 , we did this for each of the parameters by minimising a similar error function to that in Equation (5.45), and in doing so, the temperature dependences of the carbon dioxide–nitrogen parameters were found.

These were:

$$a_{\text{N}_2}(T) = 25.8842 - 55.39T + 29.6505T^2 \quad (5.46)$$

$$b_{\text{N}_2}(T) = -82.7613 + 179.897T - 97.8833T^2 \quad (5.47)$$

$$c_{\text{N}_2}(T) = 20.1581 - 33.1472T + 12.5615T^2 \quad (5.48)$$

$$d_{\text{N}_2}(T) = -43.3875 + 93.347T - 50.3857T^2 \quad (5.49)$$

$$e_{\text{N}_2}(T) = 12.249 - 26.6624T + 14.3552T^2 \quad (5.50)$$

$$f_{\text{N}_2}(T) = 326.012 - 704.801T + 381.364T^2 \quad (5.51)$$

$$g_{\text{N}_2}(T) = -281.263 + 607.427T - 328.147T^2 \quad (5.52)$$

$$a_{\text{CO}_2, \text{N}_2}(T) = 954.634 - 2070.54T + 1122.05T^2 \quad (5.53)$$

$$b_{\text{CO}_2, \text{N}_2}(T) = -619.712 + 1349.86T - 733.905T^2 \quad (5.54)$$

$$c_{\text{CO}_2, \text{N}_2}(T) = -145.516 + 317.986T - 172.507T^2 \quad (5.55)$$

$$d_{\text{CO}_2, \text{N}_2}(T) = -1970.24 + 4269.39T - 2310.74T^2 \quad (5.56)$$

$$e_{\text{CO}_2, \text{N}_2}(T) = 2838.05 - 6137.84T + 3314.23T^2 \quad (5.57)$$

$$f_{\text{CO}_2, \text{N}_2}(T) = -244.155 + 532.828T - 290.023T^2 \quad (5.58)$$

$$g_{\text{CO}_2, \text{N}_2}(T) = 134.094 - 293.271T + 160.111T^2 \quad (5.59)$$

We can see from the following two (randomly chosen) examples how these temperature dependences resembled the parameter values at the chosen three temperature points.

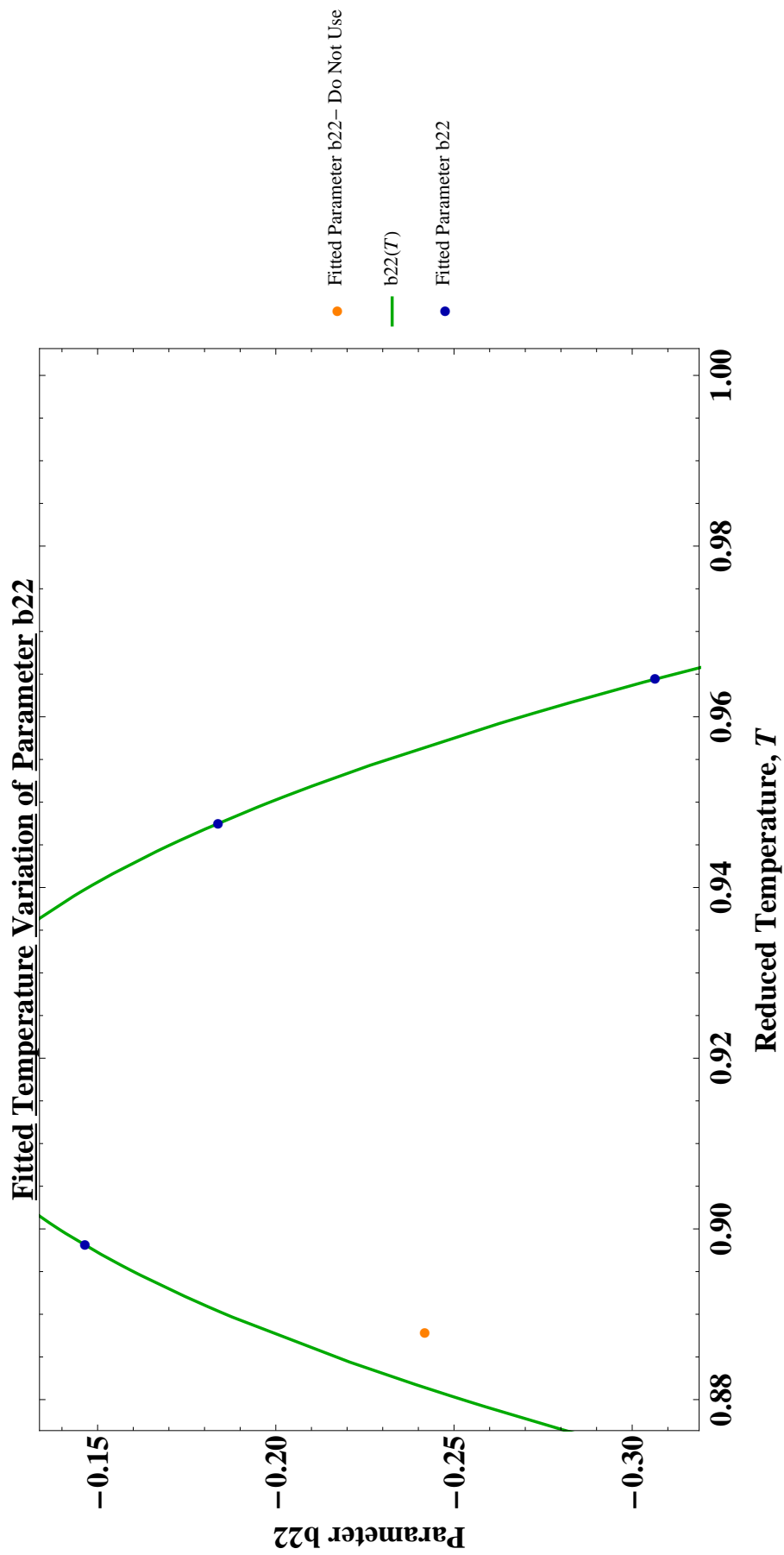


Figure 5.1: Temperature dependence for the pure nitrogen parameter b_{N_2} (denoted in the graph by b_{22})

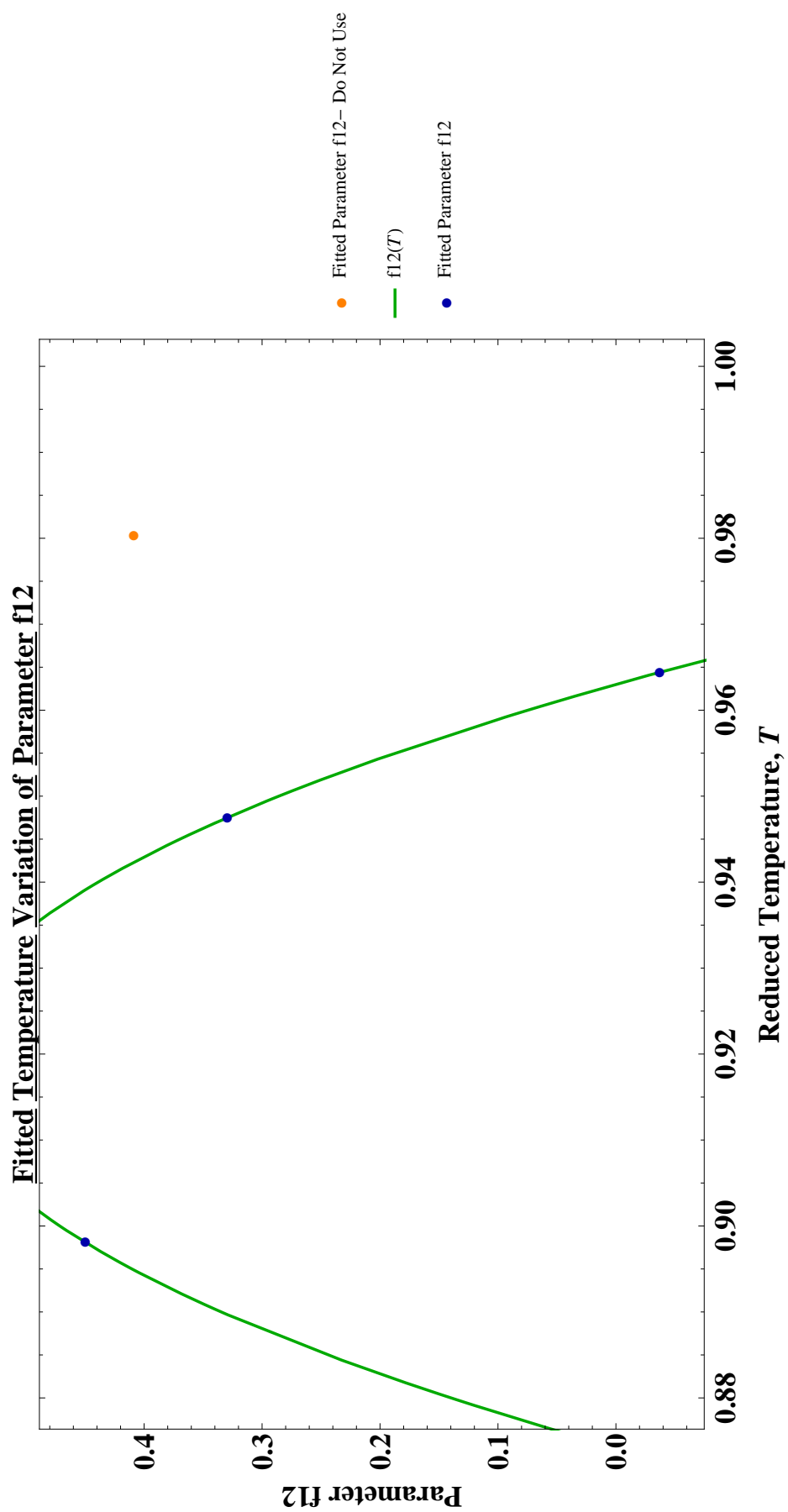


Figure 5.2: Temperature dependence for the binary interaction parameter $d_{\text{CO}_2, \text{N}_2}$ (denoted in the graph by f_{12})

5.3.5 Performance of the Full Model for Binary Mixtures of Carbon Dioxide and Nitrogen

With the model thus fully defined for the binary system involving carbon dioxide and nitrogen, we were able to assess its performance. We did this in the first instance by comparing the completed model to the same data which had been used to generate the fitted parameters. We then checked the performance of the model at temperatures where no data existed, so as to assess the behaviour as users of the model might experience it. We note that since for the nitrogen model we fit the model parameters between 273.15K and 293.3K, we would not have expected any meaningful descriptions to be given outside this range of temperatures.

We began by comparing the behaviour of the completed model to the homogeneous volume–pressure data at 273.15K.

| Nitrogen Composition (%) | Maximum Error (%) | Average Error (%) |
|----------------------------|-------------------|-------------------|
| 2.6 (liquid phase) | 9.20 | 2.75 |
| 5.0 (liquid phase) | 4.34 | 1.75 |
| 6.7 (liquid phase) | 0.87 | 0.31 |
| 5.8 (vapour phase) | 1.76 | 0.39 |
| 8.8 (vapour phase) | 2.49 | 0.59 |
| 50.8 (supercritical phase) | 4.83 | 2.30 |
| 100 | 3.73 | 1.77 |
| ALL | 9.20 | 1.79 |

Table 5.4: Pressure performance of model at 273.15

We also compared the behaviour of our model to the VLE data at the same temperature.

| Quantity | Maximum Error (%) | Average Error (%) |
|--|-------------------|-------------------|
| v_{BP} † | 0.99 | 0.53 |
| v_{DP} † | 5.72 | 3.21 |
| x_{N_2} † | 0.96 | 0.48 |
| y_{N_2} † | 6.94 | 3.64 |
| ALL | 6.94 | 1.96 |
| † where convergence to a meaningful solution had been possible | | |

Table 5.5: VLE performance of model at 273.15K

We noted the excellent performance of the model at this temperature, as compared with the literature data and volume estimations that were used to calibrate the model before smoothing of the parameters with temperature. In particular, nearly all the predictions met our target accuracy. We also highlight that the best performance of our model occurred at the liquid saturation curve (bubble curve), which we understand to be the more relevant consideration for CCS pipelines. Overall, this represented an excellent performance of our model at this temperature. Additionally, we were able to verify in Figure 5.3 that the behaviour of our model was consistent with the density data.

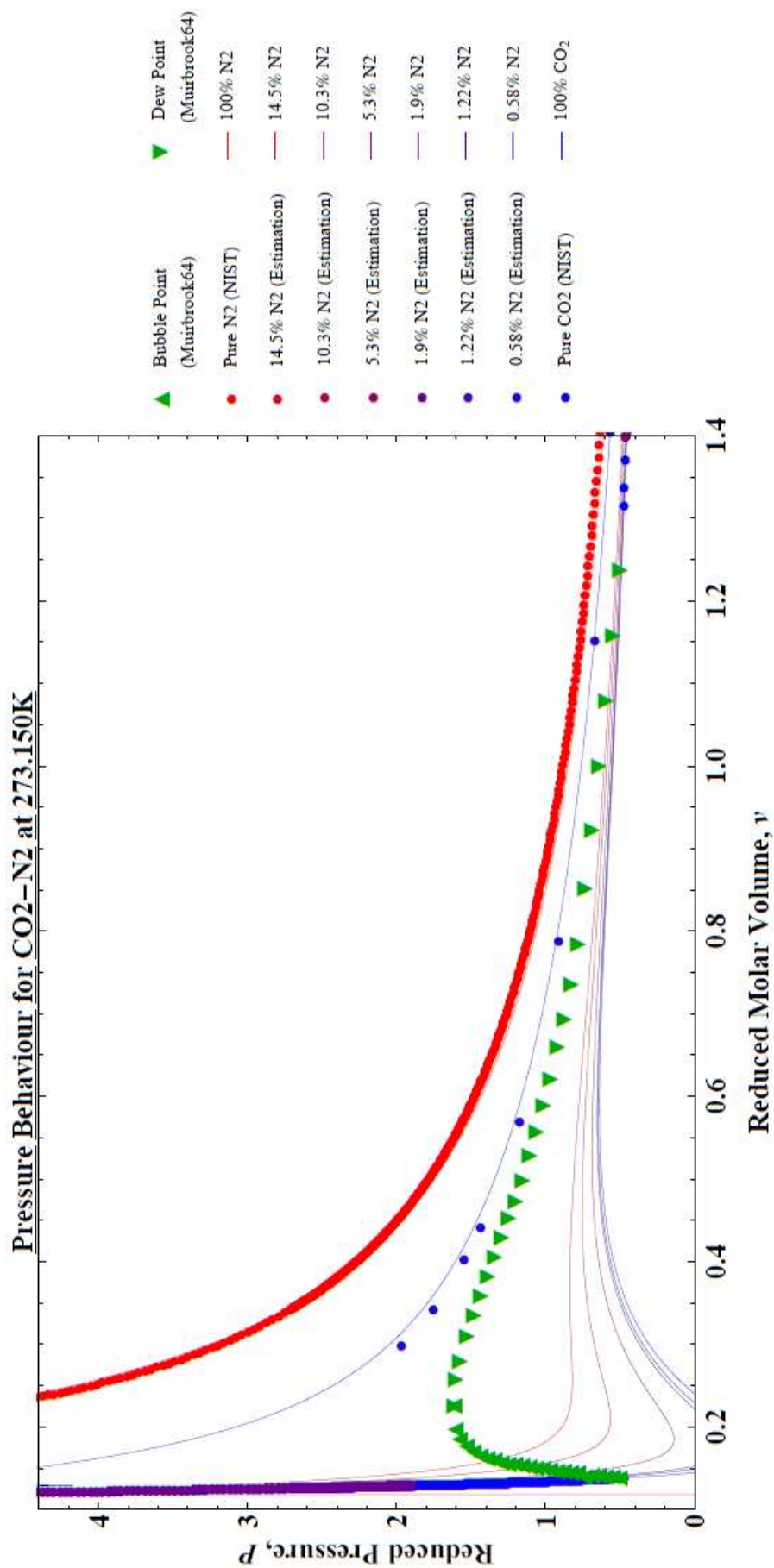


Figure 5.3: Pressure performance of model at 273.15K for carbon dioxide–nitrogen. The thin lines are the density predictions of our model with the more red lines indicating a higher concentration of nitrogen

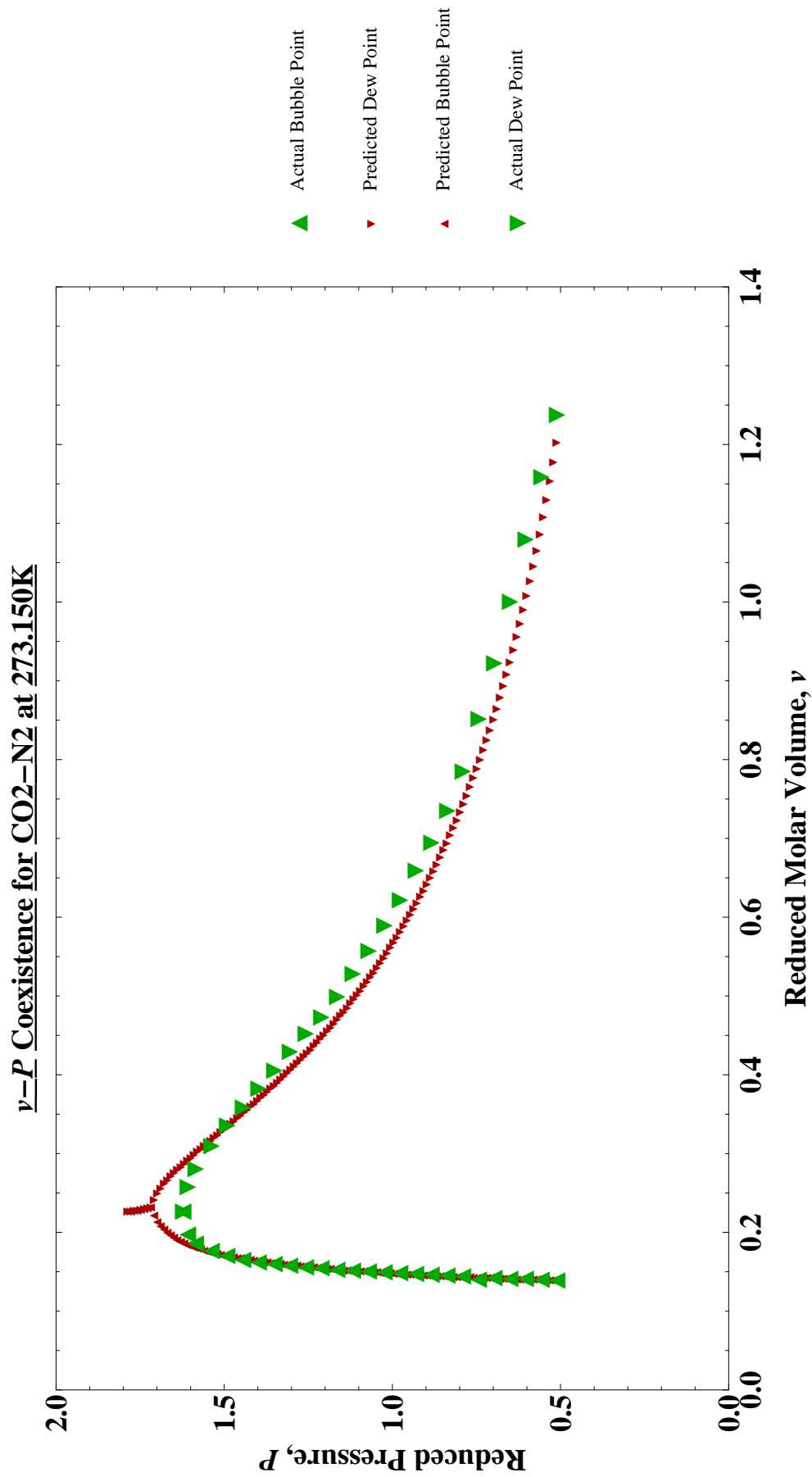


Figure 5.4: VLE coexisting volume performance of model at 273.15K for carbon dioxide–nitrogen. Note that in the interests of not over crowding this plot we do not include equivalent plots for the GERG on the basis that it is not user–friendly enough to be compared here, and we do not include the PREos on the basis that its errors in the mixture case are high

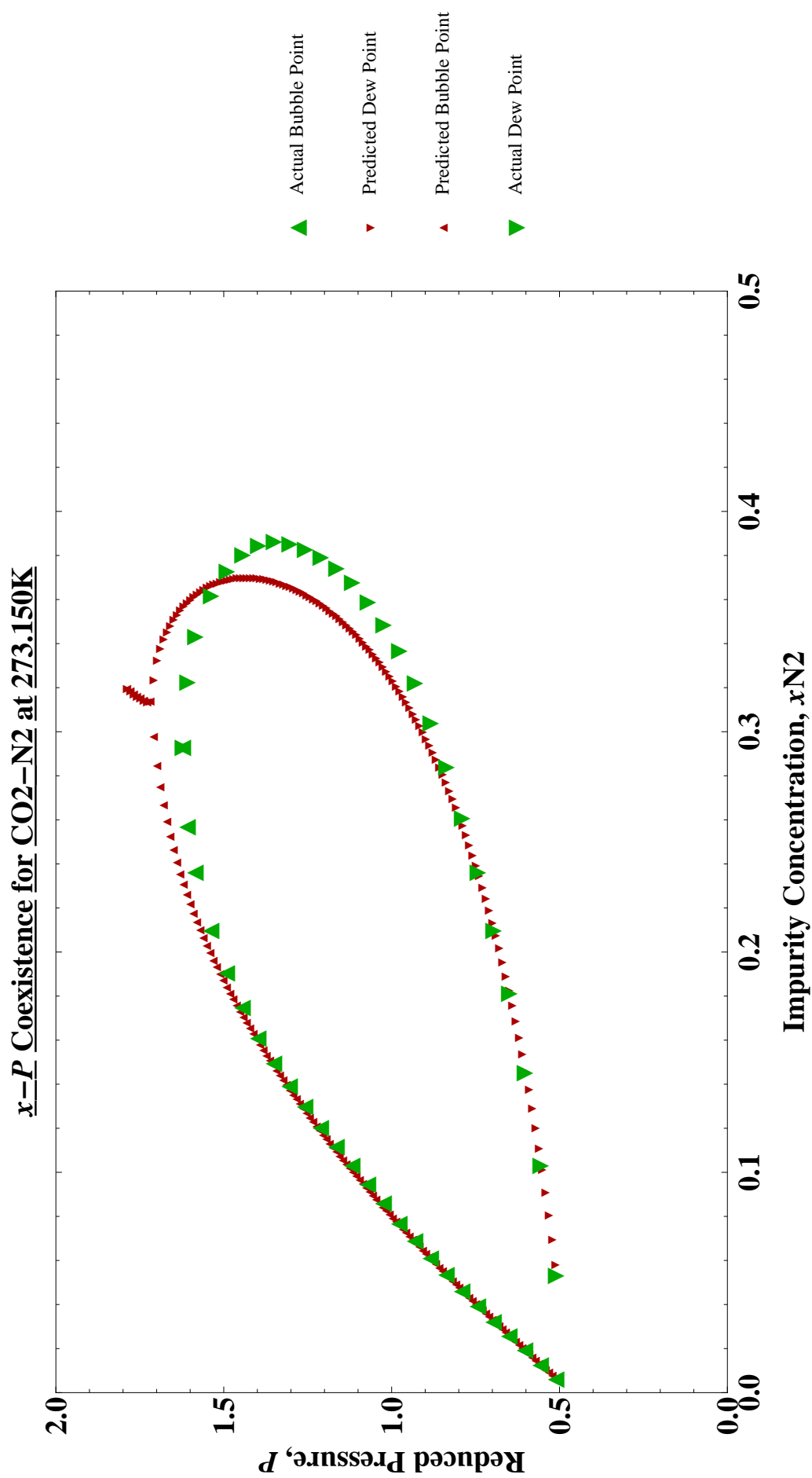


Figure 5.5: VLE coexisting mole fraction performance of model at 273.15K for carbon dioxide–nitrogen. The small “tail” at the top of the envelope is where the numerical search algorithms did not find a solution in the homogeneous region, as expected

We then compared the behaviour of our model to the homogeneous volume–pressure and composition–pressure data at 288.15K.

| Nitrogen Composition (%) | Maximum Error (%) | Average Error (%) |
|----------------------------|-------------------|-------------------|
| 3.59 (liquid phase) | 4.63 | 2.07 |
| 5.5 (liquid phase) | 9.55 | 2.58 |
| 6.01 (liquid phase) | 8.53 | 5.84 |
| 13.1 (vapour phase) | 2.67 | 0.58 |
| 18.8 (vapour phase) | 5.64 | 1.05 |
| 29.8 (supercritical phase) | 8.14 | 1.99 |
| 100 | 3.96 | 2.03 |
| ALL | 9.55 | 2.97 |

Table 5.6: Pressure performance of model at 288.15K

We also compared the behaviour of our model to the VLE data at 288.15K:

| Quantity | Maximum Error (%) | Average Error (%) |
|-------------|-------------------|-------------------|
| v_{BP} † | 1.64 | 1.22 |
| v_{DP} † | 22.21 | 11.44 |
| x_{N_2} † | 2.24 | 1.14 |
| y_{N_2} † | 8.04 | 4.12 |
| ALL | 22.21 | 4.48 |

† where convergence to a meaningful solution had been possible

Table 5.7: VLE performance of model at 288.15K

The performance of the model at higher temperature was similarly excellent to that at 273.15K. We highlight the excellent agreement with the vapour phase pressure data and again that there was a particularly good performance of our model at the liquid saturation line. In visually checking the behaviour of the model in Figures 5.6 to 5.8, we see that at this point of the temperature range, the carbon dioxide–nitrogen model behaves very well. In Figures 5.9 to 5.11 we also include plots demonstrating the behaviour of our model at 293.3K, showing that it also exhibits very strong predictions there as well. Furthermore, we include in Figures 5.12 and 5.13 the VLE behaviour of the model at 298.15K, even though this was outside the range of fitting. These highlight the robustness of the model in predicting physical properties throughout a considerable temperature range. Figure 5.14 compares the VLE behaviour of the model at a range of temperatures.

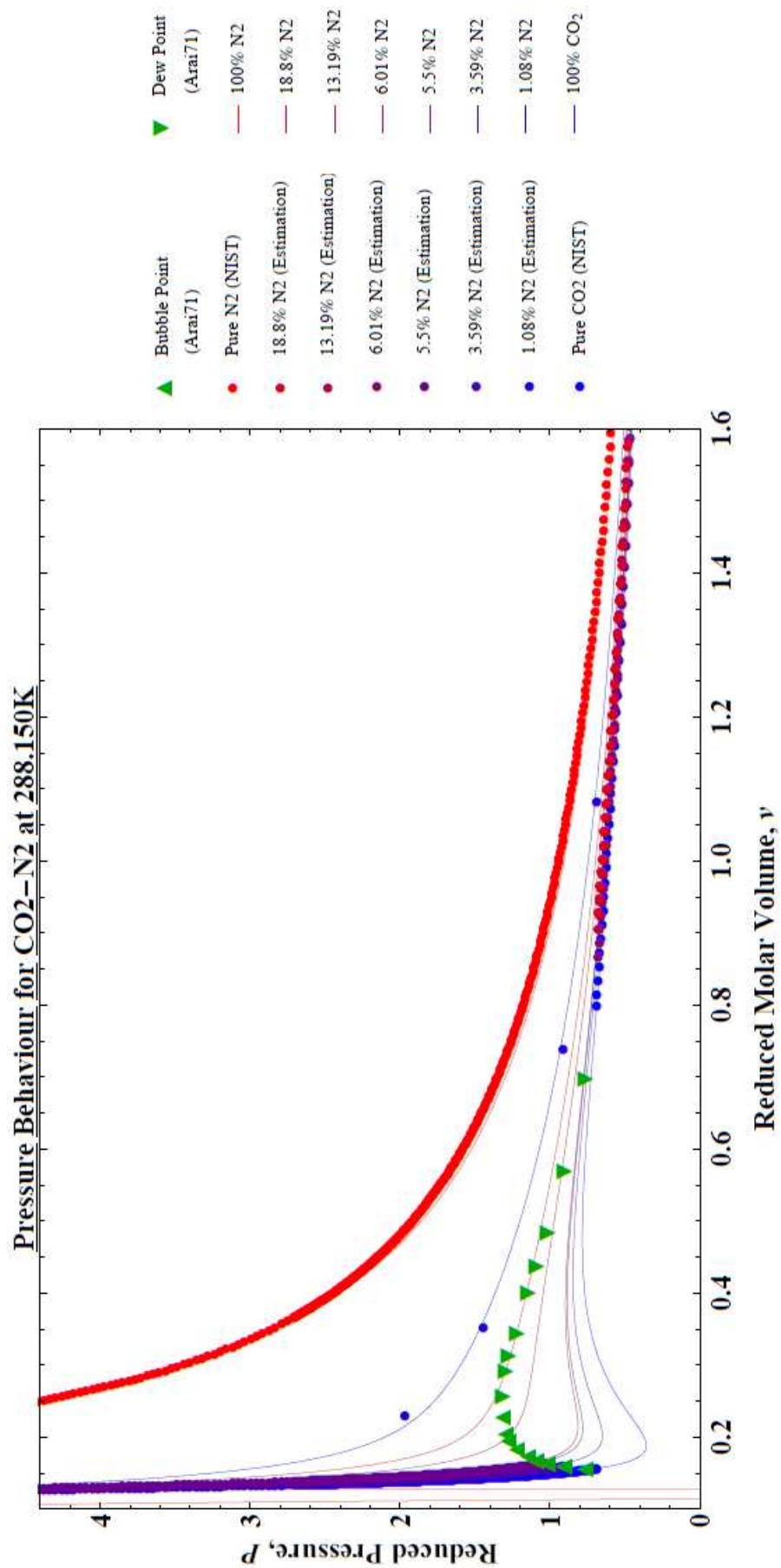


Figure 5.6: Pressure performance of model at 288.15K for carbon dioxide–nitrogen

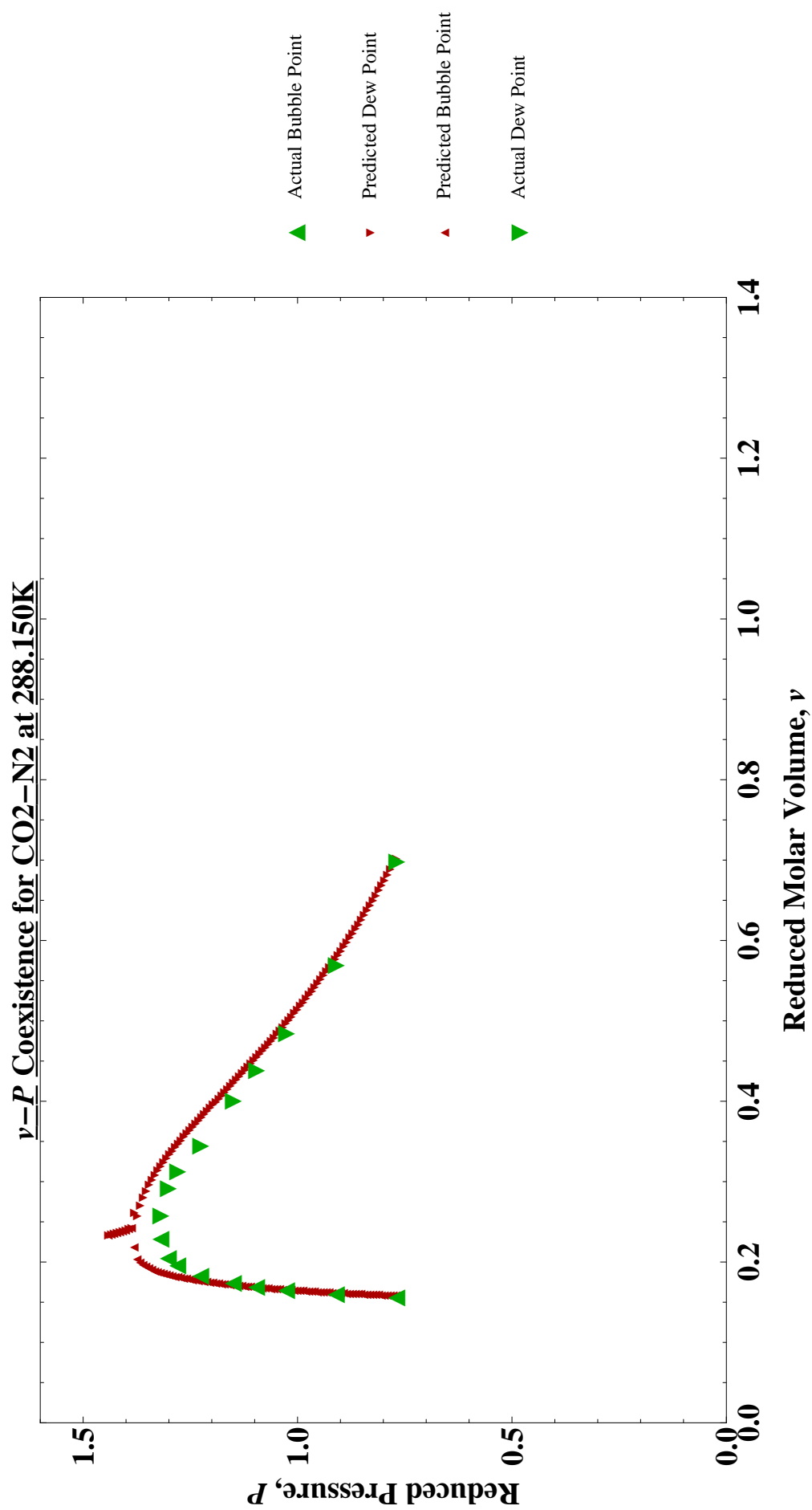


Figure 5.7: VLE coexisting volume performance of model at 288.15K for carbon dioxide–nitrogen

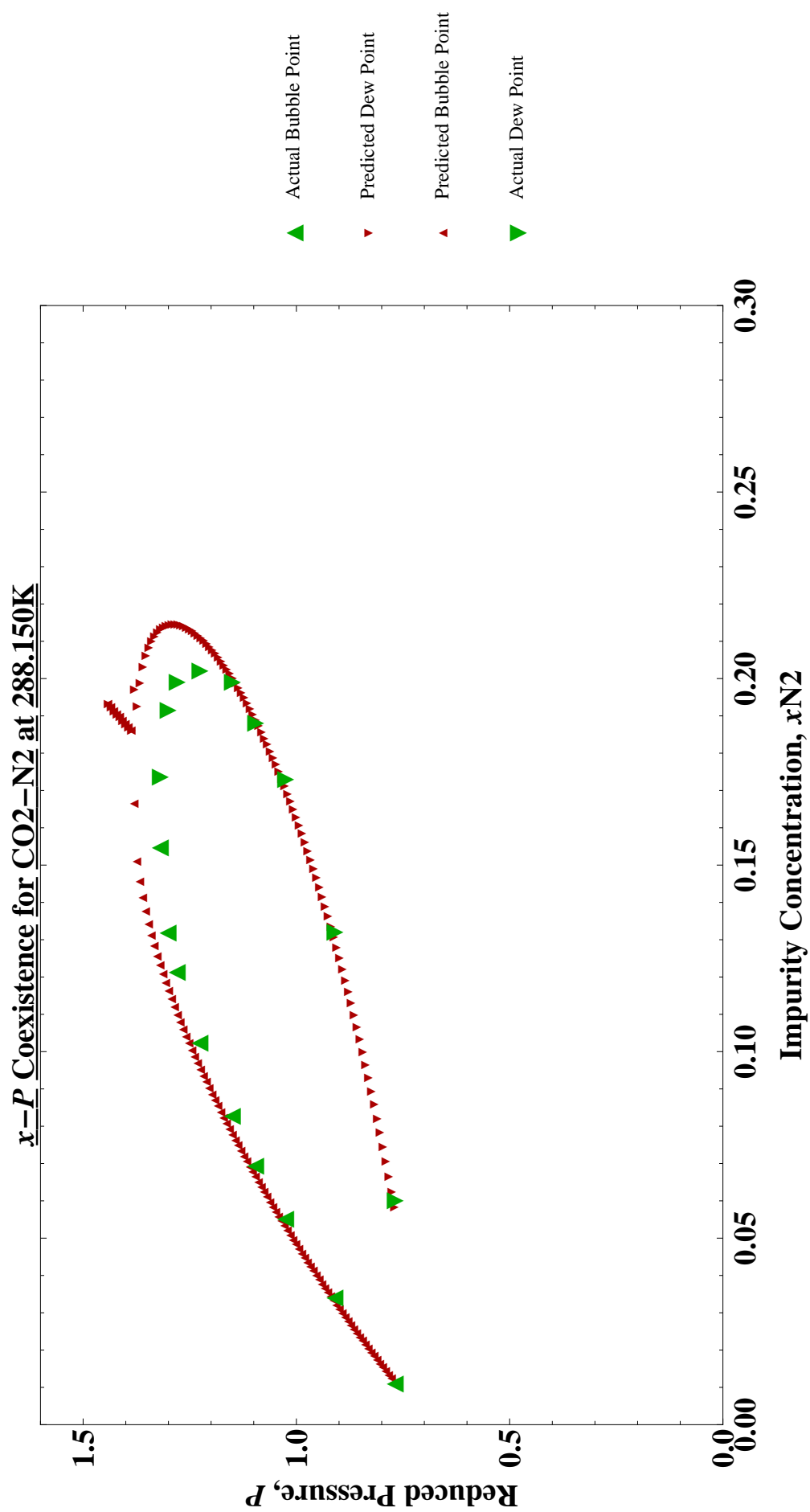


Figure 5.8: VLE coexisting mole fraction performance of model at 288.15K for carbon dioxide–nitrogen

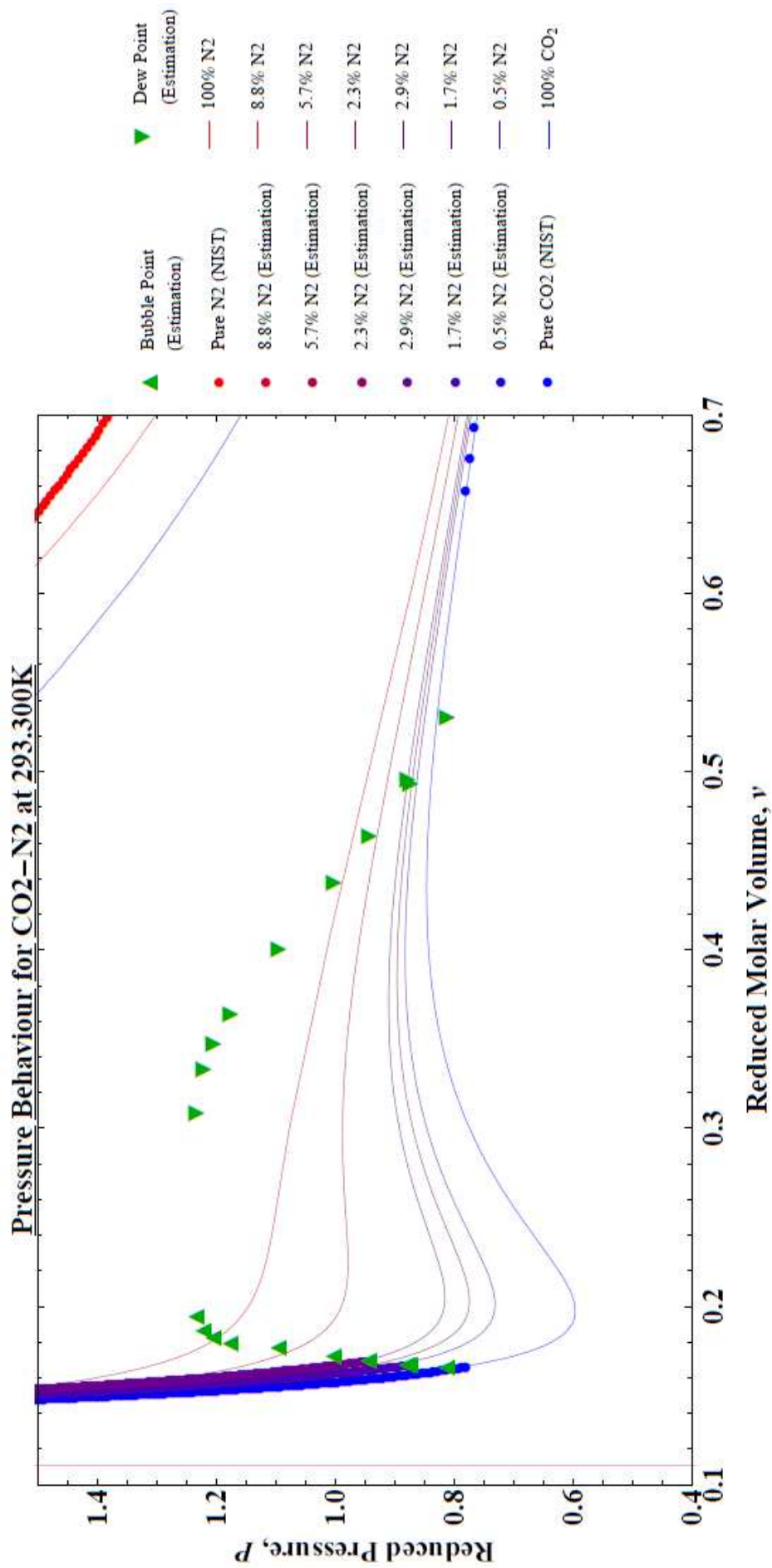


Figure 5.9: Pressure performance of model at 293.3K for carbon dioxide-nitrogen

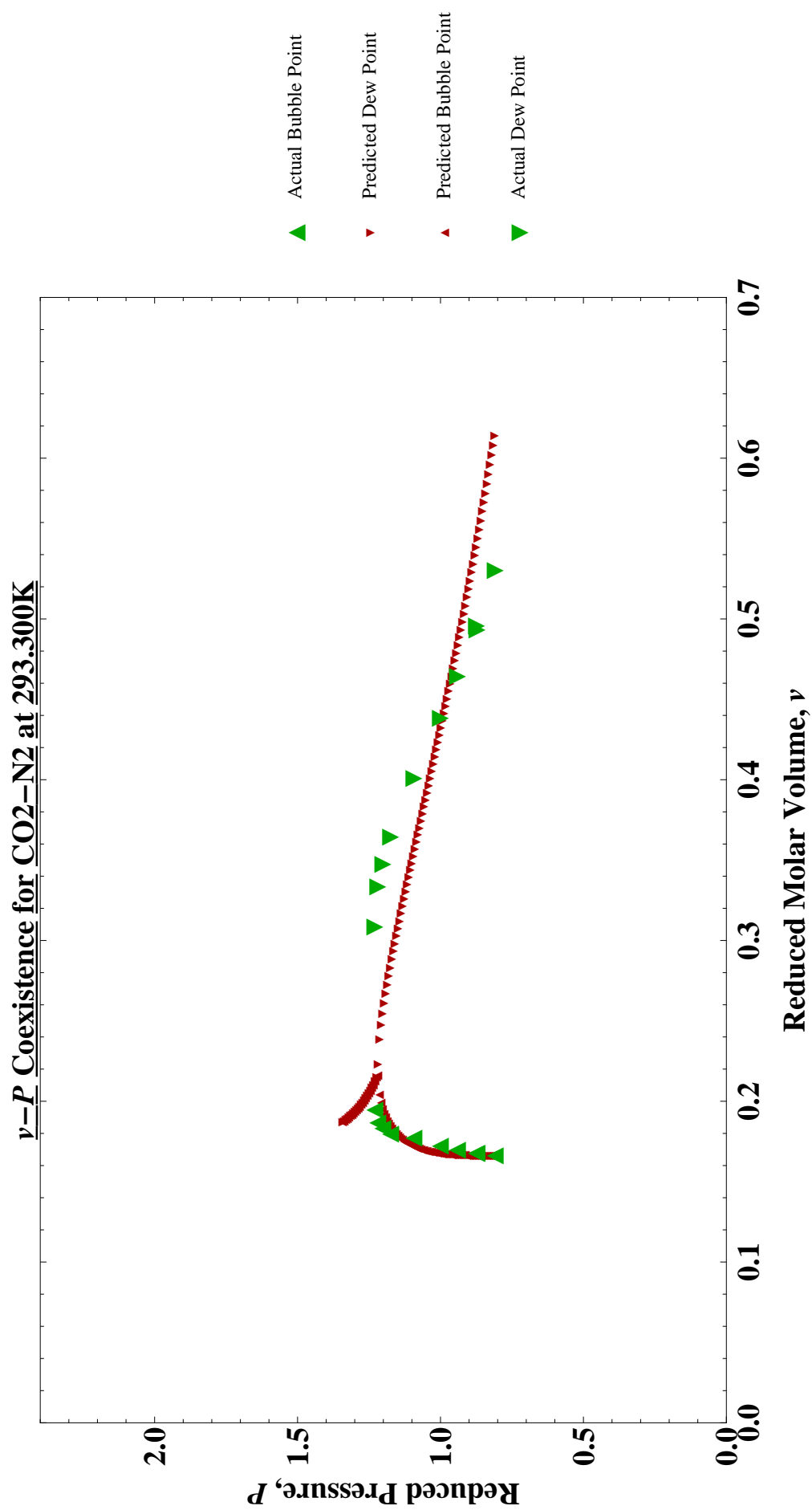


Figure 5.10: VLE coexisting volume performance of model at 293.3K for carbon dioxide–nitrogen

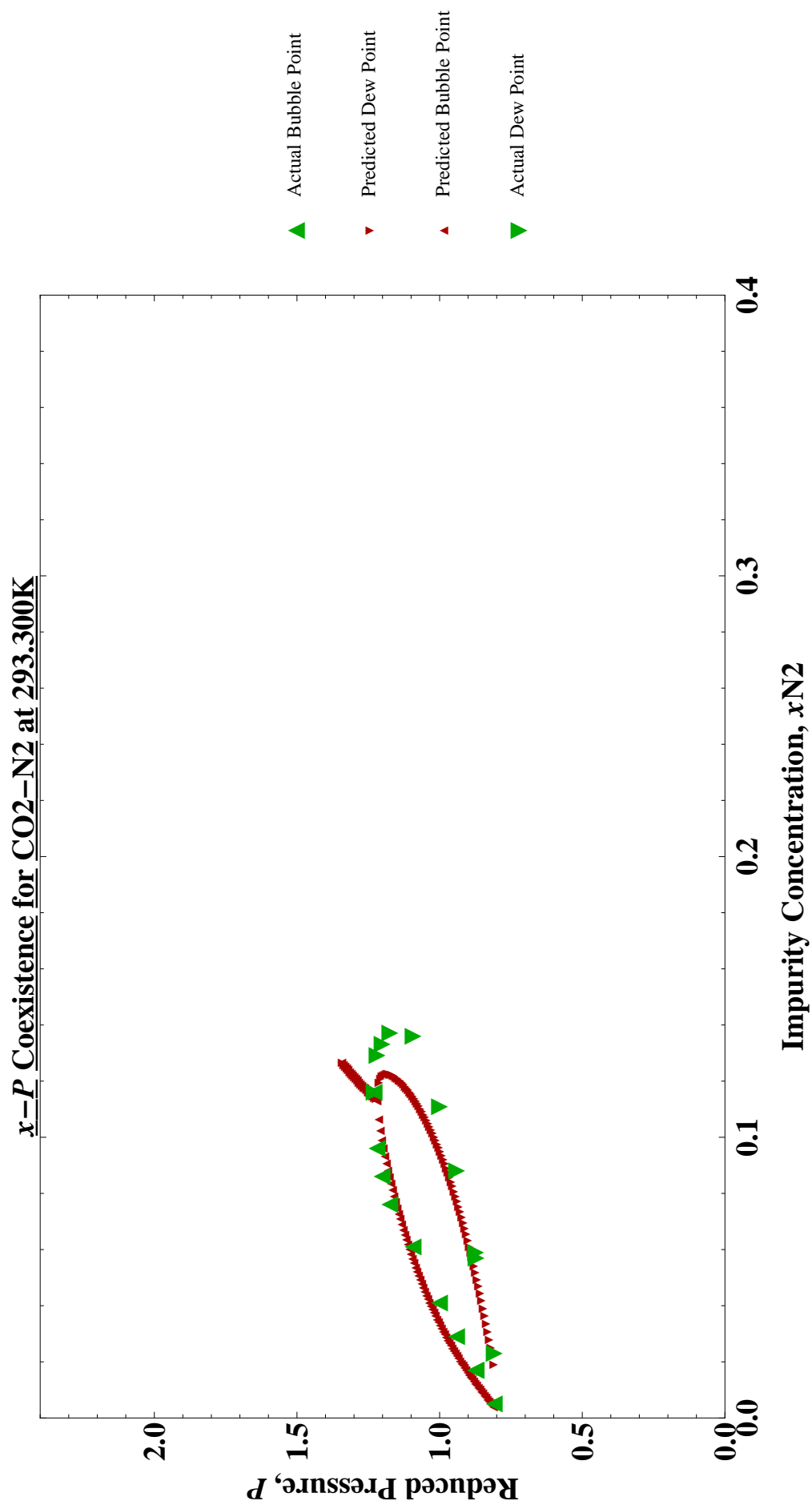


Figure 5.11: VLE coexisting mole fraction performance of model at 293.3K for carbon dioxide–nitrogen

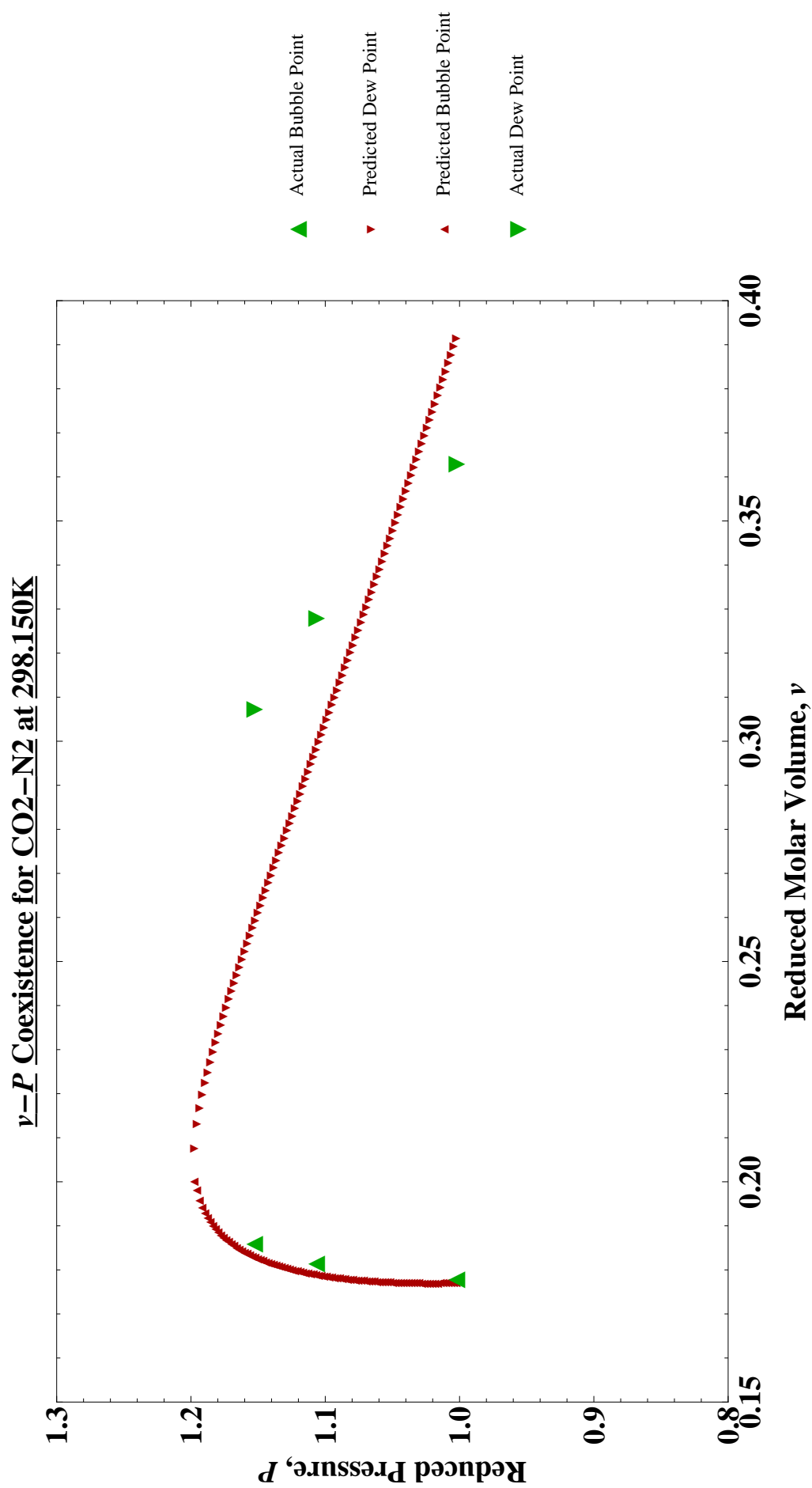


Figure 5.12: VLE coexisting volume performance of model at 298.15K for carbon dioxide–nitrogen

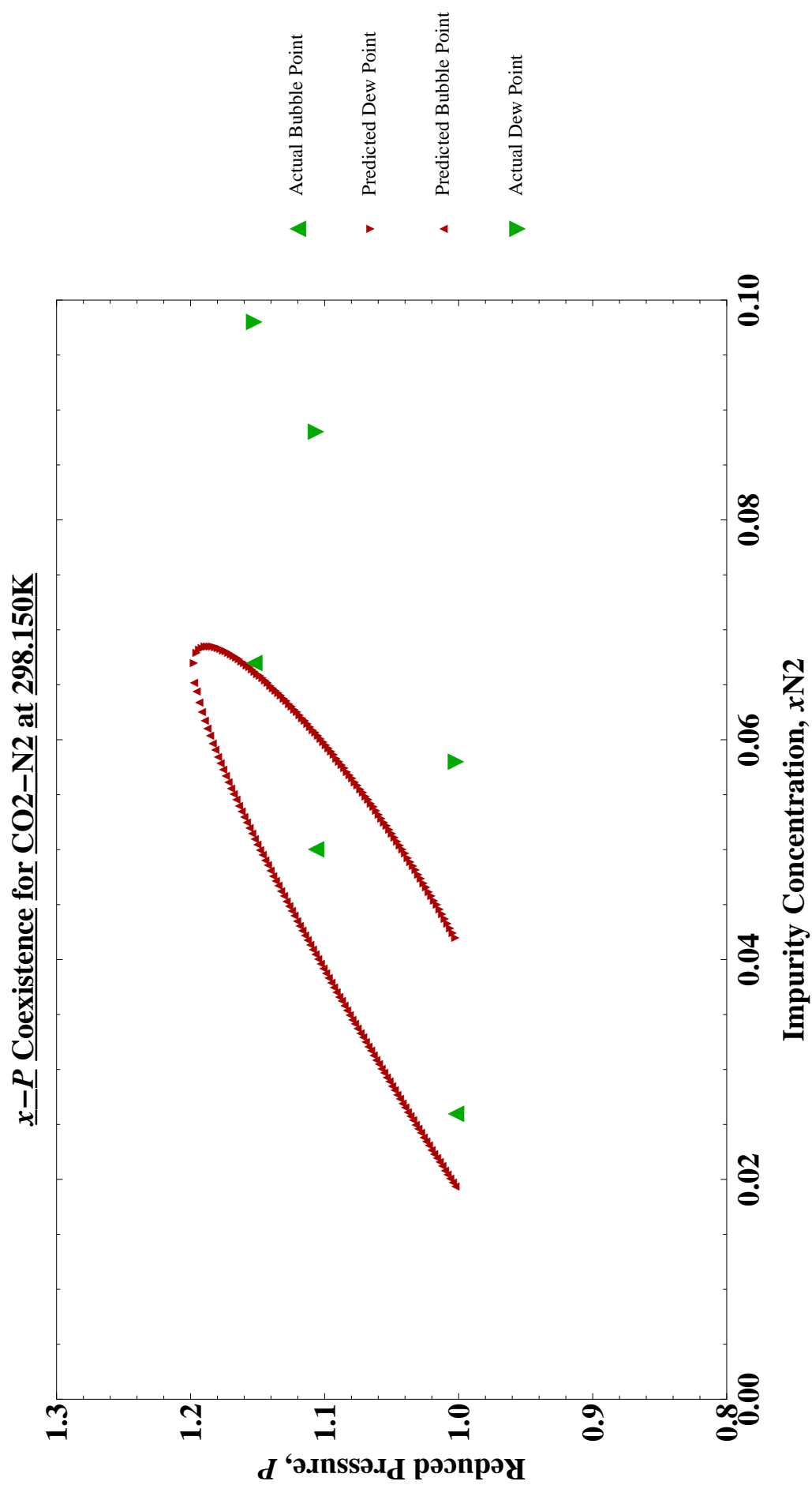


Figure 5.13: VLE coexisting mole fraction performance of model at 298.15K for carbon dioxide–nitrogen. Note that since the phase envelope is very small at this temperature, the prediction made here actually represents a very small absolute error

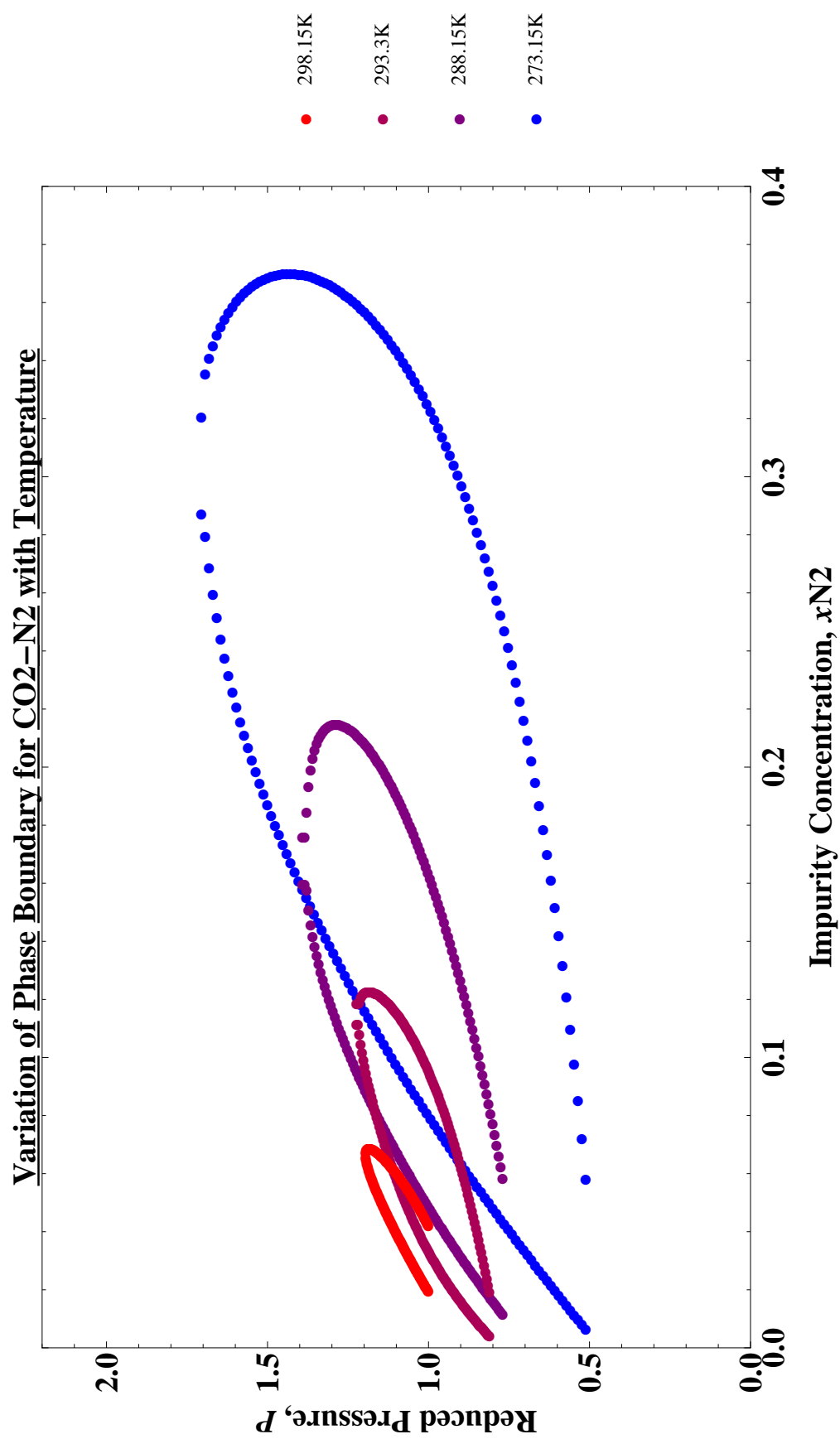


Figure 5.14: Effect of temperature on phase behaviour in the carbon dioxide–nitrogen binary system

There were numerous positives to draw from our fitting to the carbon dioxide–nitrogen data; not least the excellent pressure behaviour of the model at all nitrogen concentrations and temperatures, specifically those in the range of relevance to CCS as specified in Table 1.2. Phase behaviour predictions were also found to be well within the targets. Furthermore, use of our model to calculate the effect of temperature on the carbon dioxide–nitrogen phase boundary was possible, as shown in Figure 5.14.

Overall, for this mixture, we felt that the great promise shown by the model in the pure carbon dioxide case had been borne out. Even though the availability of the required data to affect a comprehensive fitting for a large range of temperatures was low, that data which was available together with the estimation methods had allowed us to calibrate the model in such a way as to demonstrate its true abilities.

We specifically highlight this as being a great success for the model as it proves beyond doubt that when appropriate data exists, it has the ability to give a very true description of it. We felt that if data at more temperatures became available, this would allow for an improved fit at a wider range of temperatures.

5.4 Carbon Dioxide–Hydrogen Binary Mixture

5.4.1 Data Availability

We again open this section by noting the availability of literature data for us to use in fitting the CO₂–H₂ model. There was not a single temperature at which both homogeneous pressure–density and VLE data, whether containing volumes or not, existed. This proved particularly problematic as it meant that even with our method of volume estimation, we did not have the full required amount of data in order to perform the fitting. This motivated our method of homogeneous phase density estimations.

A tabulated summary of the relevant available data is given in Table 5.8, again ordered by temperature. The availability of data in the hydrogen case was even more limited than in that of nitrogen. We can see from Table 5.8 that there were just two temperature points where complete VLE data existed: at 273.15K [92] and 258.15K [92], which is below the relevant range of temperatures for CCS pipelines. In addition, there were no temperatures at which VLE data and homogeneous density data existed. Whereas for the nitrogen case where there were some, albeit not many, temperatures at which both data types existed, for the hydrogen case, this

created a scenario in which without the estimation techniques described in Chapter 2, we would have been unable to perform a single fitting. With these methods however, we were able to build the model around seven temperature points accounting for the validity of some of the data presented, whilst ensuring we covered the correct temperature range; 298.15K, 290K, 280K, 273.15K, 270K, 260K, and the data at 258.15K, which even though we acknowledge is below our range of interest, since it was the full array of VLE data, by including it in our considerations, we hoped it may anchor the model and give some extra accuracy at lower temperatures.

| Temperature (K) | Homogeneous Density Data Sources | VLE Data Sources |
|---|----------------------------------|------------------|
| 258.15 | | [92] |
| 260 | | [110] † |
| 270 | | [110] † |
| 273.15 | | [92] [84] † |
| 278.15 | | [90] † |
| 280 | | [110] † |
| 288.15 | [111] | |
| 290 | | [110] † |
| 290.15 | | [90] † |
| 293.15 | [111] | |
| 298.15 | | [90] † |
| 303.15 | [111] | |
| † means the VLE data in this source did not contain volumes | | |

Table 5.8: A summary of available data by source for carbon dioxide–hydrogen binary mixtures

5.4.2 Fitting the Carbon Dioxide–Hydrogen Binary Model Parameters

For fitting the carbon dioxide–hydrogen parameters, we proceeded in exactly the same way as for fitting the nitrogen parameters discussed in Section 5.3. We first determined the pure hydrogen parameters a_{H_2} through g_{H_2} at the seven temperature points specified by temporarily introducing a linear mixing rule similar to that given in Equation (5.44), and minimising the error function which found the values of the parameters best describing the two types of data. Again, this was done by simulated annealing at 298.15K and local minimisation at all subsequent temperatures. To find the binary interaction parameters we reintroduced the quadratic mixing rules and carried out the same process.

For finding the pure hydrogen parameters we again set $W = 0.99$ in the error function to persuade the fitting regime to concentrate on finding a good fit for the homogeneous density data to begin with. We again set $W = 0.05$ for finding the binary interaction parameters to force these to influence the search algorithm to focus on fitting the VLE behaviour more carefully.

For the pure hydrogen parameters and the binary interaction parameters of this system, the values we found by following this method are as summarised in Table 5.9.

| $T(K)$ | a_{H_2} | b_{H_2} | c_{H_2} | d_{H_2} | e_{H_2} | f_{H_2} | g_{H_2} |
|--------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 298.15 | -0.036120 | -0.268687 | -0.140686 | 0.000064 | -0.342518 | 0.841807 | -0.570231 |
| 290 | -0.001527 | -0.115780 | -0.010731 | -0.041427 | -0.341615 | 0.532446 | -0.283406 |
| 280 | -0.010139 | -0.203360 | -0.000606 | -0.039236 | -0.350992 | 0.449553 | -0.202573 |
| 273.15 | -0.016366 | -0.285983 | 0.044472 | -0.071323 | -0.358931 | 0.668197 | -0.354539 |
| 270 | -0.036633 | -0.261411 | 0.066326 | -0.061539 | -0.359609 | 0.666215 | -0.395087 |
| 260 | -0.025148 | -0.241830 | 0.061862 | -0.064112 | -0.356514 | 0.607538 | -0.338173 |
| 258.15 | 0.033329 | -0.150848 | -0.052928 | 0.087893 | -0.835536 | 0.458757 | -0.205049 |

| $T(K)$ | a_{CO_2, H_2} | b_{CO_2, H_2} | c_{CO_2, H_2} | d_{CO_2, H_2} | e_{CO_2, H_2} | f_{CO_2, H_2} | g_{CO_2, H_2} |
|--------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 298.15 | 1.020390 | -0.599860 | -0.714769 | -0.200111 | 0.071537 | 0.994452 | -0.543545 |
| 290 | 23.672552 | -1.137099 | -0.851500 | -0.818970 | -1.247985 | 4.546853 | -3.464147 |
| 280 | 0.925204 | 0.031172 | -0.125157 | -0.220122 | 0.070576 | 1.052079 | -0.534298 |
| 273.15 | 0.764031 | -0.247773 | -0.943430 | -0.776950 | 0.062453 | 1.681050 | -1.033491 |
| 270 | 0.768990 | -0.409059 | -1.083002 | -0.754101 | -1.147136 | 1.675058 | -1.037449 |
| 260 | 0.620573 | -0.518750 | -1.029732 | -0.651093 | -0.989265 | 1.378729 | -1.474389 |
| 258.15 | 0.810443 | -0.490394 | -0.905972 | -0.632675 | -0.172276 | 1.674597 | -1.185195 |

Table 5.9: Fitted parameter values for the carbon dioxide–hydrogen binary system

5.4.3 Preliminary Indications of Performance

After having found the fourteen parameters at each temperature point, we evaluated the performance of the proposed model to check the fitting that had been achieved through the optimisation of the error function had rendered a suitable representation of the data that was used to calibrate it in each case.

We did this by checking the percentage errors of the values suggested by our model for both the homogeneous density and VLE. A summary is in Table 5.10:

| Temperature (K) | Homogeneous Density | | v_{BP} † | | v_{DP} † | | x_{H_2} † | | y_{H_2} † | |
|--------------------|---------------------|---------|------------|---------|------------|---------|-------------|---------|-------------|---------|
| | Maximum | Average | Maximum | Average | Maximum | Average | Maximum | Average | Maximum | Average |
| 298.15 | 21.10 | 3.81 | 140.95 | 31.89 | 81.39 | 49.02 | 123.82 | 22.97 | 15.80 | 10.18 |
| 290 | 71.55 | 28.25 | 83.96 | 71.27 | 74.10 | 28.26 | 19.86 | 9.70 | 49.84 | 18.02 |
| 280 | 28.99 | 8.80 | 37.88 | 12.03 | 21.92 | 13.10 | 26.96 | 16.01 | 32.11 | 21.47 |
| 273.15 | 54.80 | 18.73 | 17.53 | 15.36 | 203.57 | 70.58 | 8.23 | 5.20 | 266.19 | 101.21 |
| 270 | 30.98 | 11.92 | 2.33 | 1.91 | 28.13 | 12.33 | 7.97 | 3.75 | 30.36 | 15.76 |
| 260 | 258.63 | 82.51 | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |
| 258.15 | 104.02 | 44.80 | 145.06 | 69.70 | 552.57 | 210.74 | 71.50 | 28.51 | 407.74 | 233.62 |

† where convergence to a meaningful solution had been possible

Table 5.10: Preliminary testing of predictions made by our model for the carbon dioxide–hydrogen binary system, with results suggesting that with smoothly varying parameters the model could be good

It is evident from these figures that where there was a lack of suitable literature data to fit the model parameters to, the model has been unable to recreate that data. Nevertheless, we decided to fit the temperature dependence of the parameters to all the temperature points apart from 260K where a particularly bad fitting had been done, and 290K as the parameter values were significantly different to those surround it.

5.4.4 Variation of Model Parameters with Temperature

We again specified a quadratic temperature dependence, as for the binary mixture involving nitrogen. Following the same procedure as before to determine these dependences, we obtained:

$$a_{\text{H}_2}(T) = 2.18375 - 4.48398T + 2.27583T^2 \quad (5.60)$$

$$b_{\text{H}_2}(T) = 8.11481 - 17.5501T + 9.19340T^2 \quad (5.61)$$

$$c_{\text{H}_2}(T) = -24.007 + 53.8038T - 30.1181T^2 \quad (5.62)$$

$$d_{\text{H}_2}(T) = 16.8885 - 36.6077T + 19.7692T^2 \quad (5.63)$$

$$e_{\text{H}_2}(T) = -46.8681 + 99.0315T - 52.6178T^2 \quad (5.64)$$

$$f_{\text{H}_2}(T) = 13.5063 - 30.4078T + 17.7652T^2 \quad (5.65)$$

$$g_{\text{H}_2}(T) = -15.1254 + 34.353T - 19.7936T^2 \quad (5.66)$$

$$a_{\text{CO}_2, \text{H}_2}(T) = 25.1402 - 54.8628T + 30.8661T^2 \quad (5.67)$$

$$b_{\text{CO}_2, \text{H}_2}(T) = -58.0063 + 127.15T - 69.9675T^2 \quad (5.68)$$

$$c_{\text{CO}_2, \text{H}_2}(T) = 20.2645 - 47.7947T + 26.924T^2 \quad (5.69)$$

$$d_{\text{CO}_2, \text{H}_2}(T) = 59.4809 - 134.987T + 75.5951T^2 \quad (5.70)$$

$$e_{\text{CO}_2, \text{H}_2}(T) = -31.1574 + 66.5051T - 35.3448T^2 \quad (5.71)$$

$$f_{\text{CO}_2, \text{H}_2}(T) = -47.6094 + 112.811T - 64.5009T^2 \quad (5.72)$$

$$g_{\text{CO}_2, \text{H}_2}(T) = 12.9232 - 35.2366T + 21.9309T^2 \quad (5.73)$$

We can see from the following two examples how these temperature dependences resembled the parameter values at the chosen five temperature points.

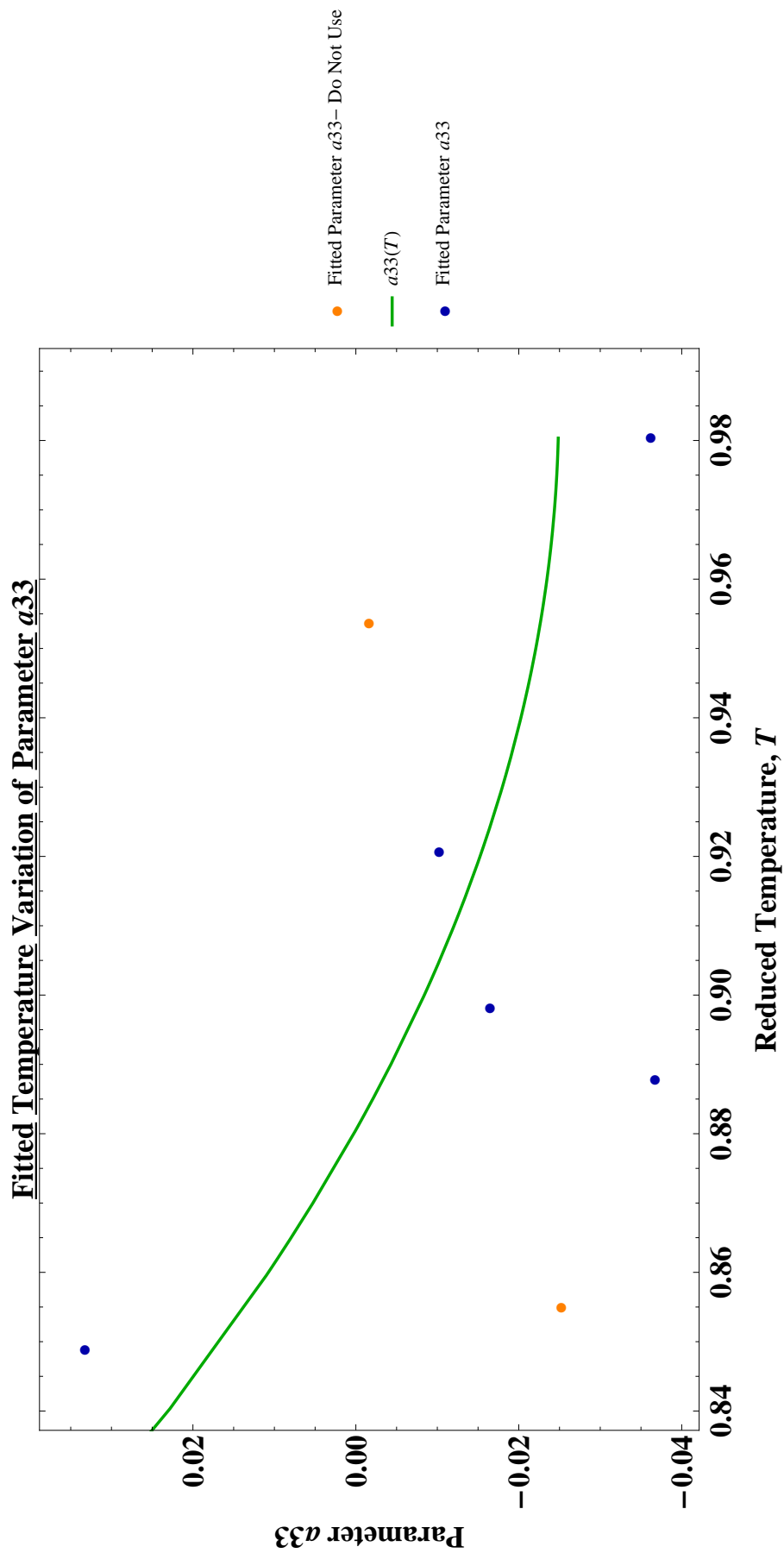


Figure 5.15: Temperature dependence for the pure nitrogen parameter a_{H_2} (denoted in the graph by a_{33})

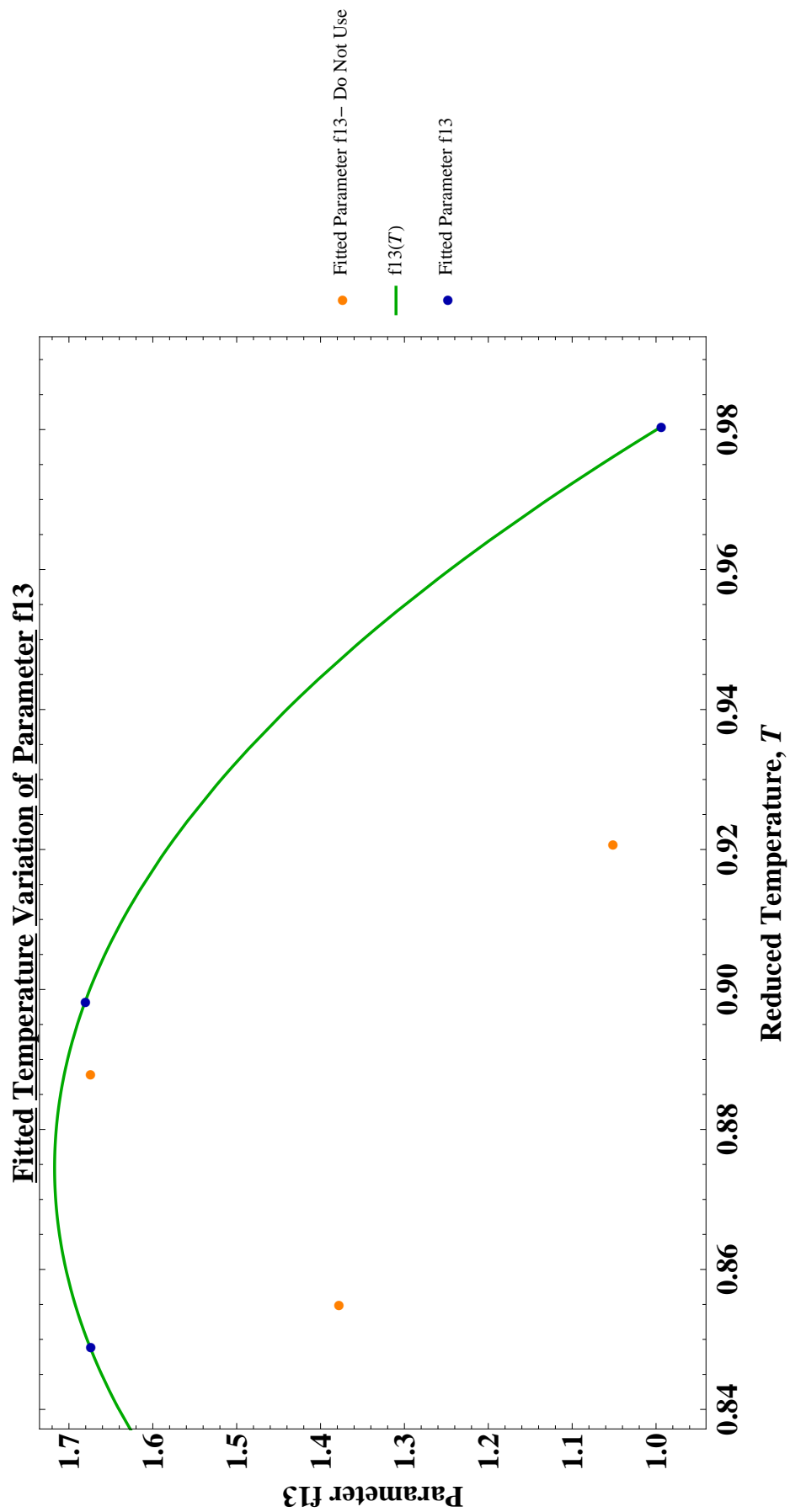


Figure 5.16: Temperature dependence for the binary interaction parameter $f_{\text{CO}_2, \text{H}_2}$ (denoted in the graph by f_{13})

5.4.5 Performance of the Full Model for Binary Mixtures of Carbon Dioxide and Hydrogen

With the model thus fully defined for the binary system involving carbon dioxide and hydrogen, we were able to assess the performance of the final model for this particular mixture. We did this by once again comparing the model at temperature points which had been used to generate the fitted parameters, and then by checking the performance at temperatures where no data existed in order to check performance there. We note that since we fit the model parameters between 258.15K and 298.15K, we would not expect meaningful descriptions to be given significantly outside this range of particular relevance to CCS pipeline operation.

We began by comparing the behaviour of our model to the homogeneous volume–pressure data at 298.15K.

| Hydrogen Composition (%) | Maximum Error (%) | Average Error (%) |
|--------------------------|-------------------|-------------------|
| 0.96 (liquid phase) | 21.15 | 5.90 |
| 2.84 (liquid phase) | 13.66 | 3.55 |
| 3.82 (liquid phase) | 15.33 | 5.50 |
| 4.25 (vapour phase) | 4.05 | 1.10 |
| 7.43 (vapour phase) | 5.97 | 1.26 |
| 10.06 (vapour phase) | 6.91 | 1.39 |
| 100 | 11.70 | 5.55 |
| ALL | 21.15 | 4.51 |

Table 5.11: Pressure performance of model at 298.15K

We also compared the behaviour of our model to the VLE data at 298.15K.

| Quantity | Maximum Error (%) | Average Error (%) |
|-------------|-------------------|-------------------|
| v_{BP} † | 10.01 | 8.31 |
| v_{DP} † | 61.70 | 52.35 |
| x_{N_2} † | 1.28 | 0.98 |
| y_{N_2} † | 3.39 | 2.02 |
| ALL | 61.70 | 15.92 |

† where convergence to a meaningful solution had been possible

Table 5.12: VLE performance of model at 298.15K

We note that with the exception of the dew curve volumes, most predictions either met our target accuracy, or were significantly better. It is worth pointing out that at this temperature we employed volume estimation for the VLE volumes, meaning that although some high percentage errors were given, these are only compared to the estimations, and not the real data. We again highlight that the best performance of our model occurred at the liquid saturation line (bubble curve), which is advantageous for application to CCS pipelines. Overall, we felt this behaviour represented an acceptable performance of our model at this temperature. We can additionally visually verify in Figures 5.17 to 5.19 that the behaviour of our model is broadly consistent with that little data which was available.

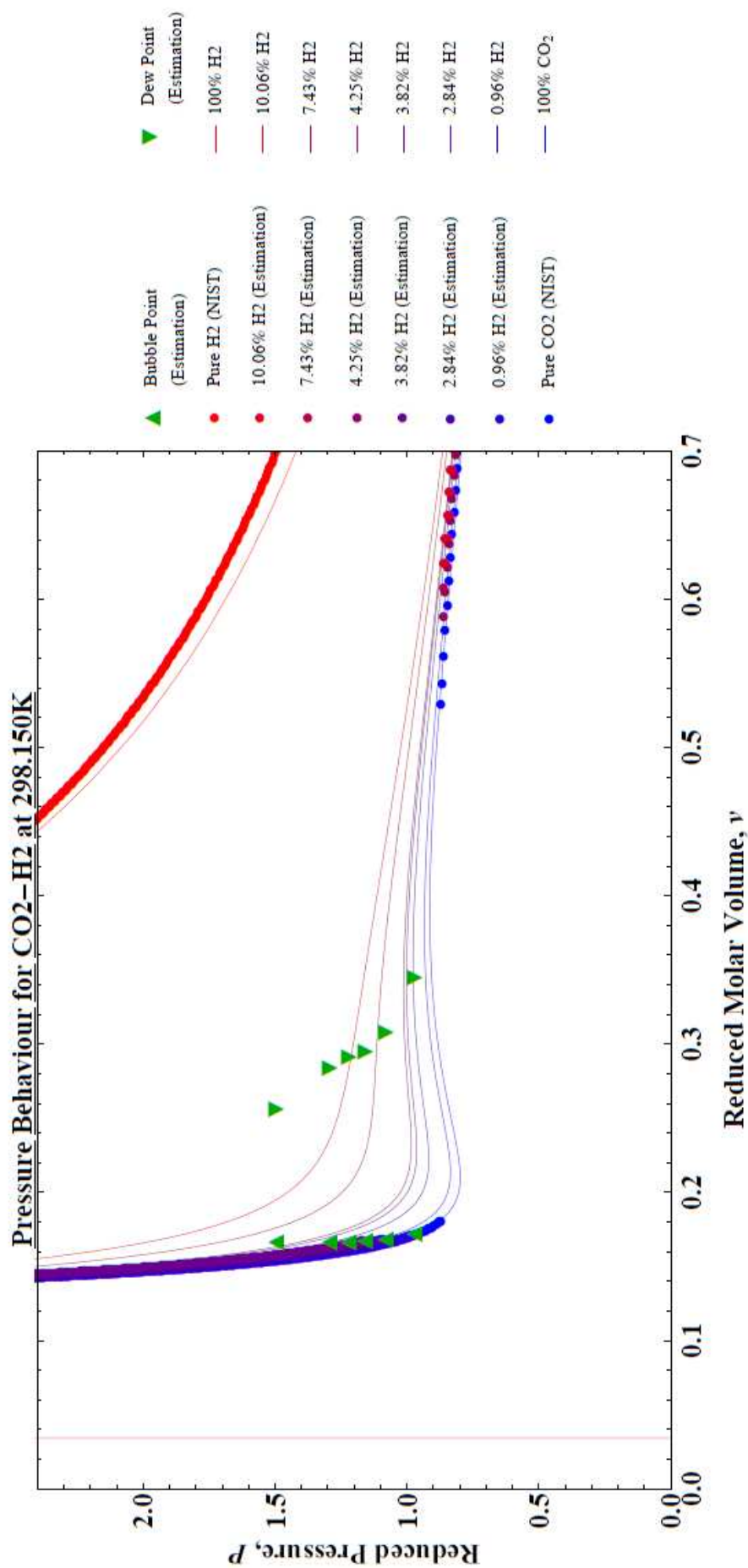


Figure 5.17: Pressure performance of model at 298.15K for carbon dioxide-hydrogen

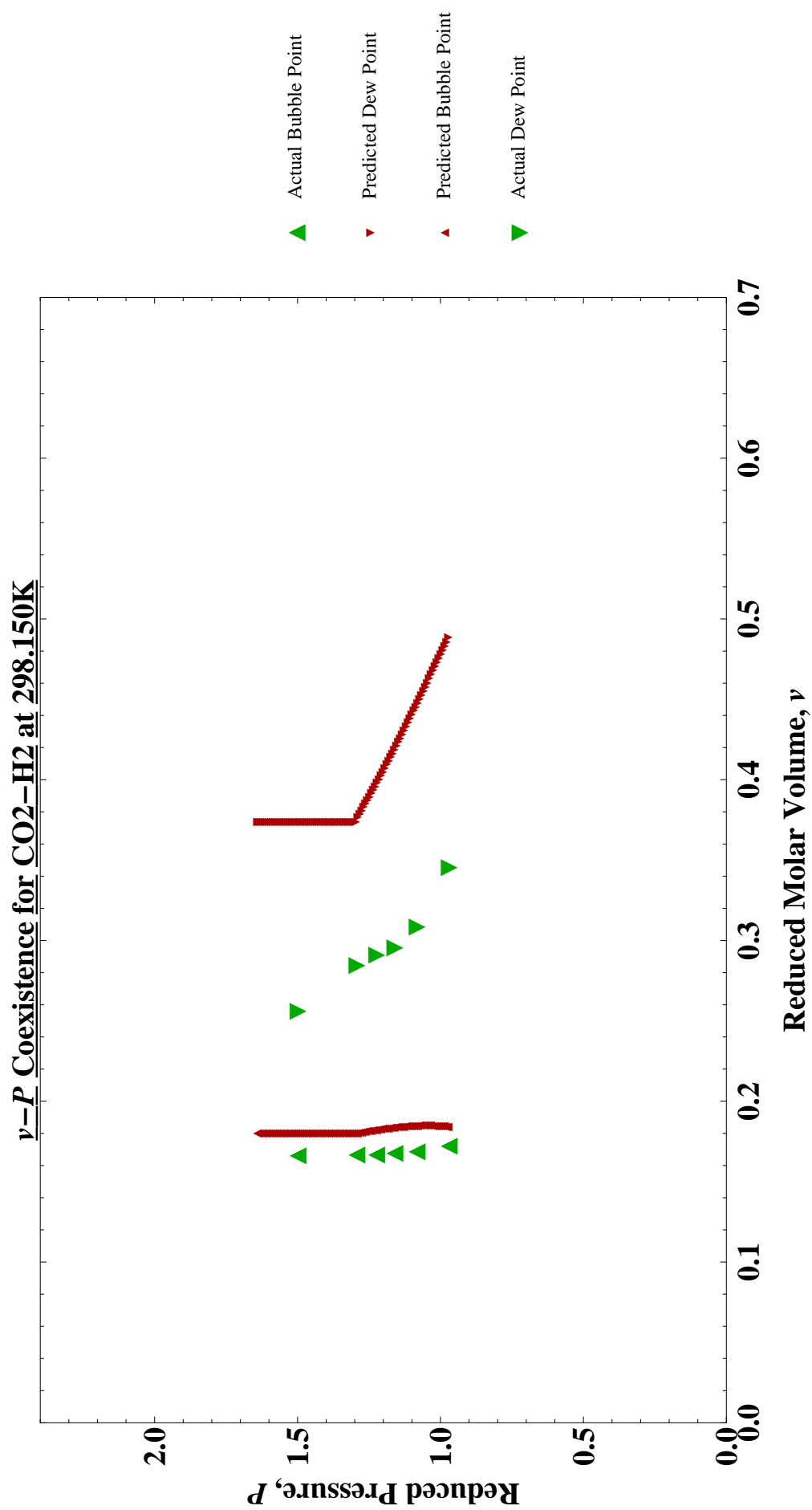


Figure 5.18: VLE coexisting volume performance of model at 298.15K for carbon dioxide-hydrogen

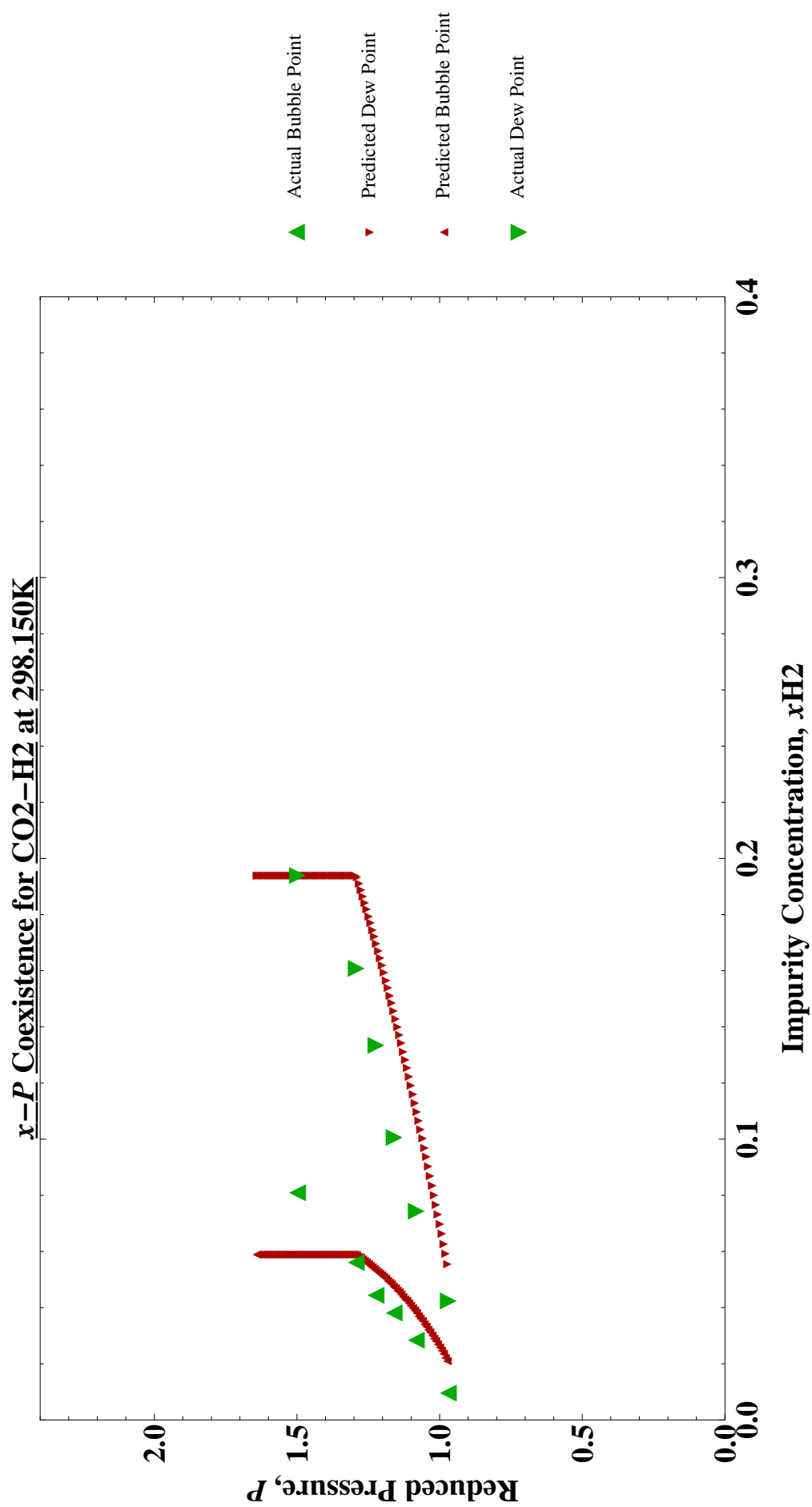


Figure 5.19: VLE coexisting mole fraction performance of model at 298.15K for carbon dioxide-hydrogen

We then compared the behaviour of our model to the homogeneous volume–pressure data at 273.15K.

| Hydrogen Composition (%) | Maximum Error (%) | Average Error (%) |
|--------------------------|-------------------|-------------------|
| 2.66 (liquid phase) | 23.06 | 16.04 |
| 7.99 (liquid phase) | 52.54 | 33.77 |
| 19.3 (liquid phase) | 35.80 | 18.78 |
| 36.15 (vapour phase) | 2.09 | 0.56 |
| 55 (vapour phase) | 1.74 | 1.23 |
| 61 (vapour phase) | 2.25 | 1.59 |
| 100 | 18.58 | 9.47 |
| ALL | 52.54 | 15.56 |

Table 5.13: Pressure performance of the model at 273.15K

We also compared the behaviour of our model to the VLE data at 273.15K:

| Quantity | Maximum Error (%) | Average Error (%) |
|-------------|-------------------|-------------------|
| v_{BP} † | 21.17 | 10.85 |
| v_{DP} † | 47.08 | 26.22 |
| x_{N_2} † | 4.83 | 2.90 |
| y_{N_2} † | 10.74 | 7.95 |
| ALL | 47.08 | 5.99 |

† where convergence to a meaningful solution had been possible

Table 5.14: VLE performance of model at 273.15K

The performance of the model at both these temperatures was a little below the standard we had been aiming for. However, in some places, particularly close to the dew curve in the homogeneous vapour phase, we found the model to give good descriptions of the data. In the liquid phase there was also a generally good pressure description. As was the case for the nitrogen binary mixture, the model gave excellent descriptions of the bubble line, either meeting the target aim or falling just outside.

We again visually checked the behaviour of the model in Figures 5.19 to 5.22 for consistency, and we saw that at low concentrations of hydrogen, as is to be anticipated for CCS pipelines, a very good description is given.

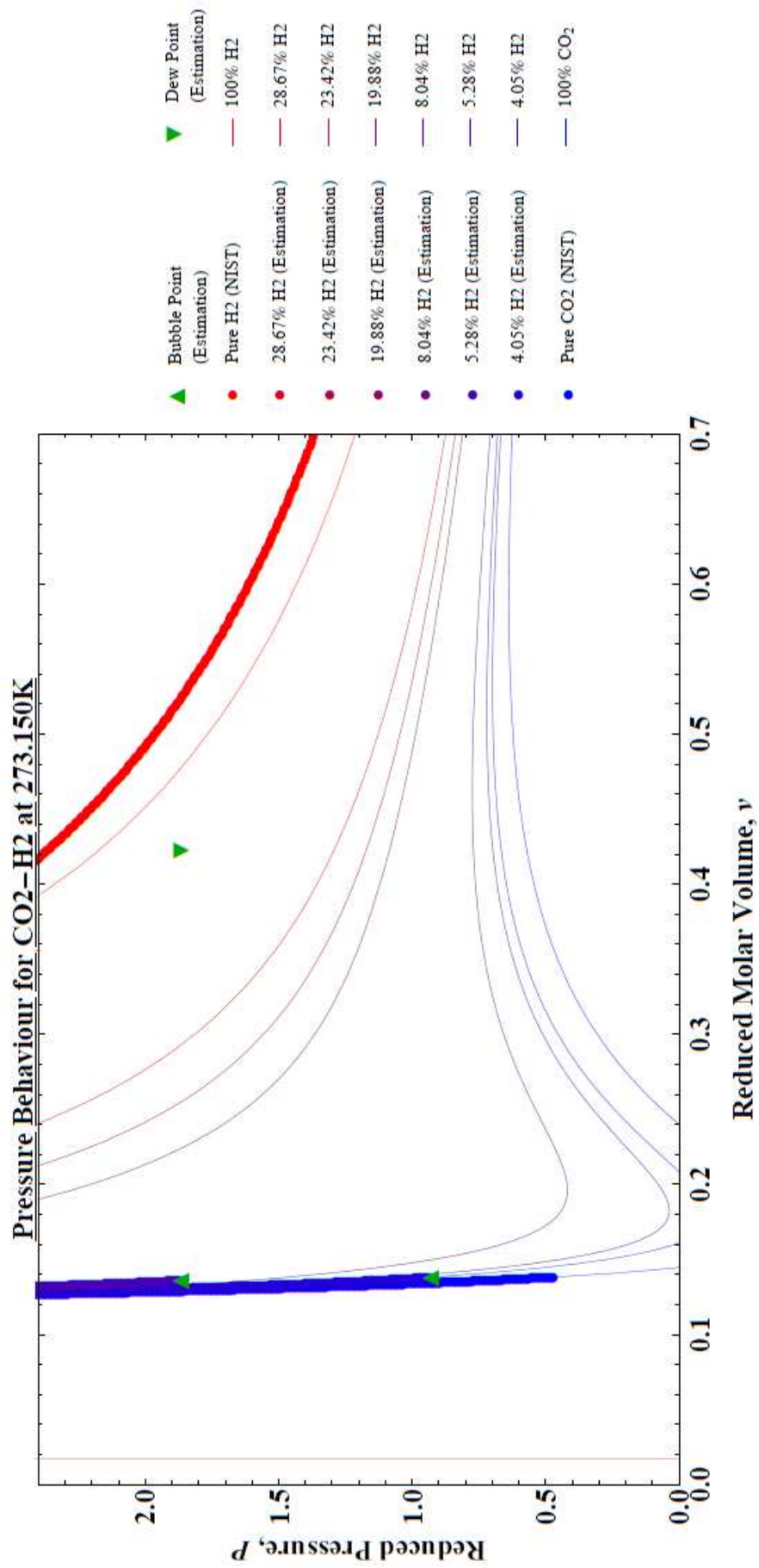


Figure 5.20: Pressure performance of model at 273.15K for carbon dioxide-hydrogen

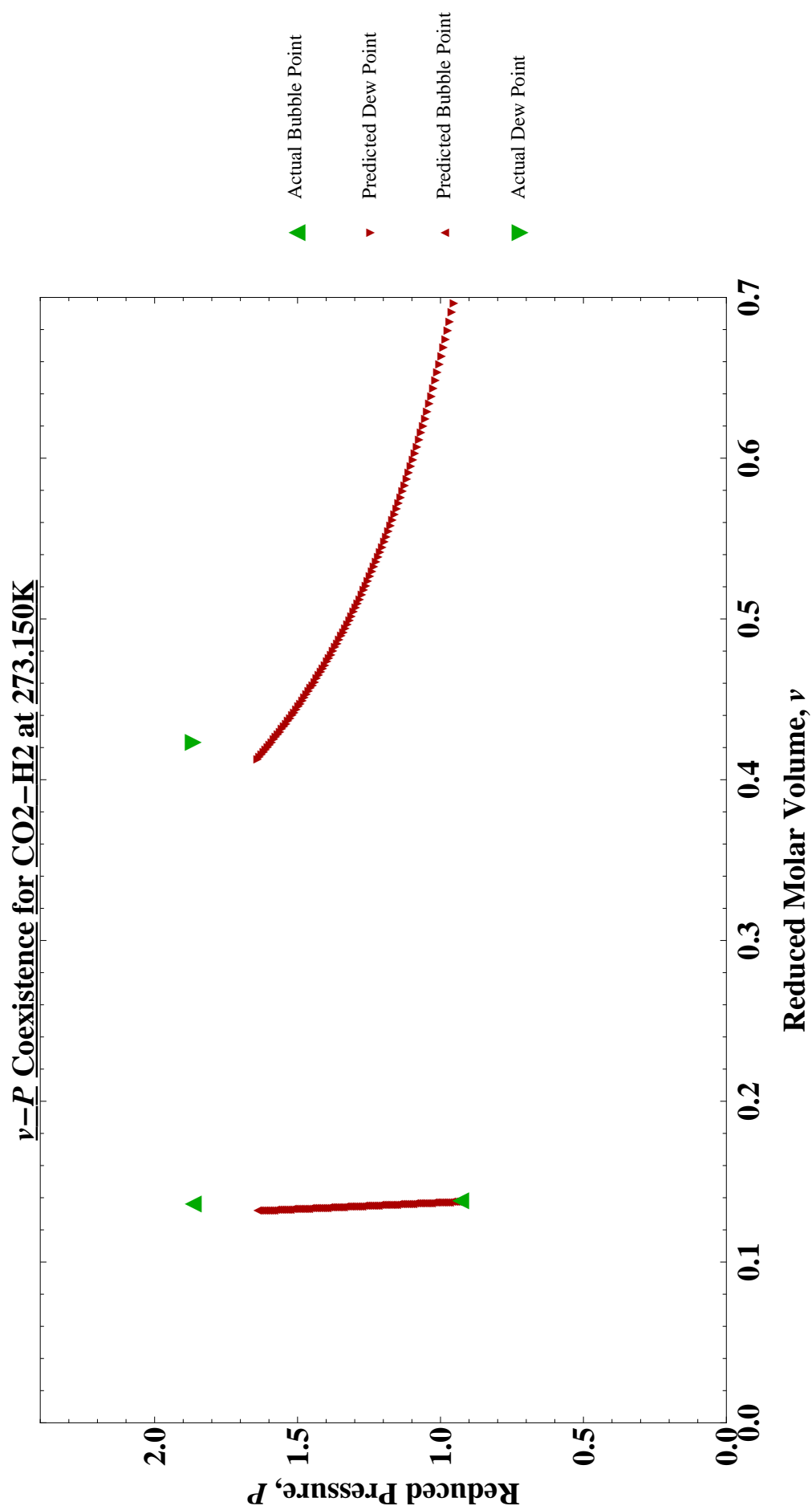


Figure 5.21: VLE coexisting volume performance of model at 273.15K for carbon dioxide-hydrogen

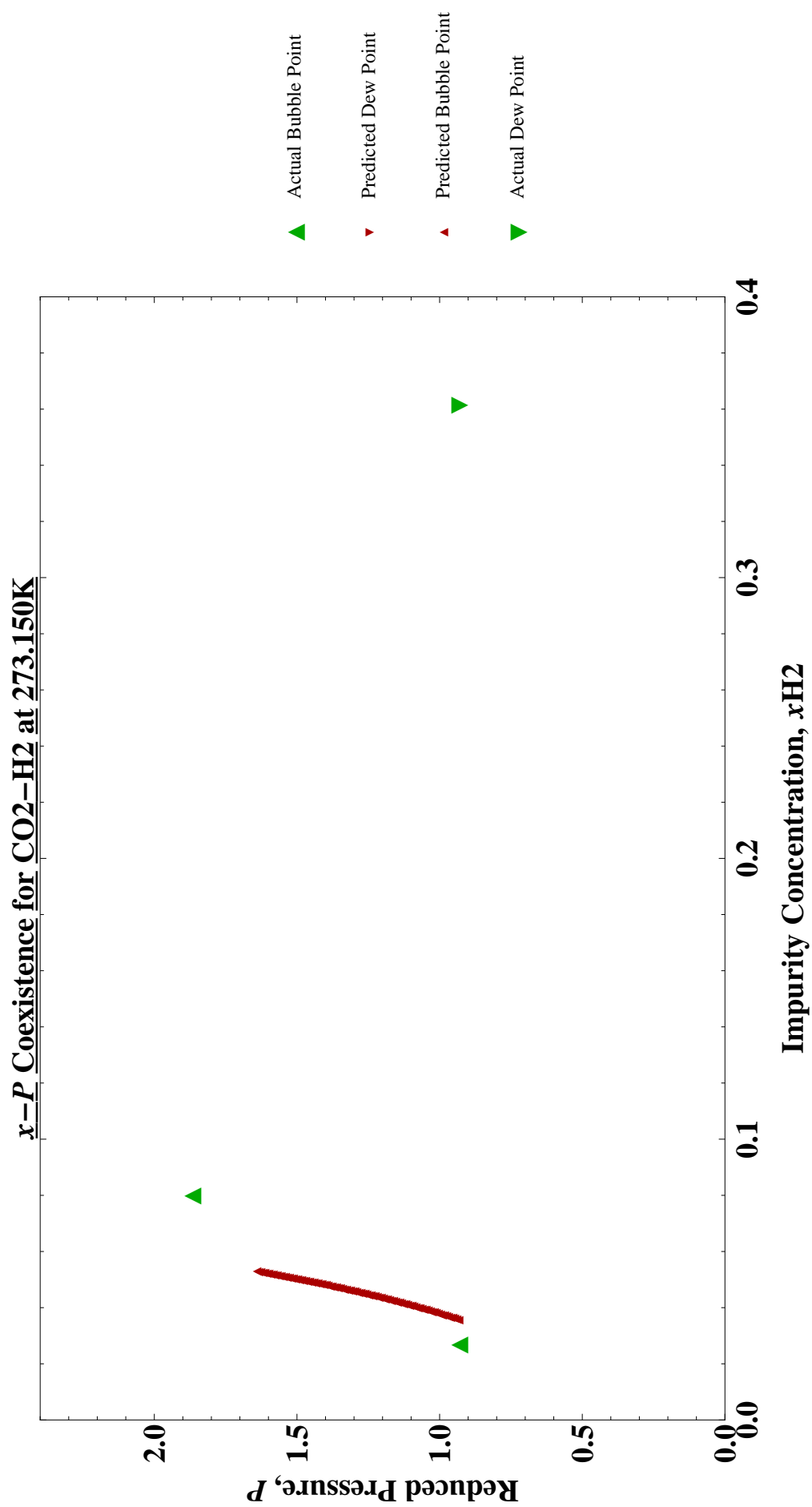


Figure 5.22: VLE coexisting mole fraction performance of model at 273.15K for carbon dioxide-hydrogen

We again suggest that where the model falls down could be a direct result of the lack of data that was available for fitting. Following on from the analyses at 298.15K and 273.15K, we also generated some plots at 285K and 275K; temperatures at which we had no data to fit to, in order to ensure consistent and physical behaviour.

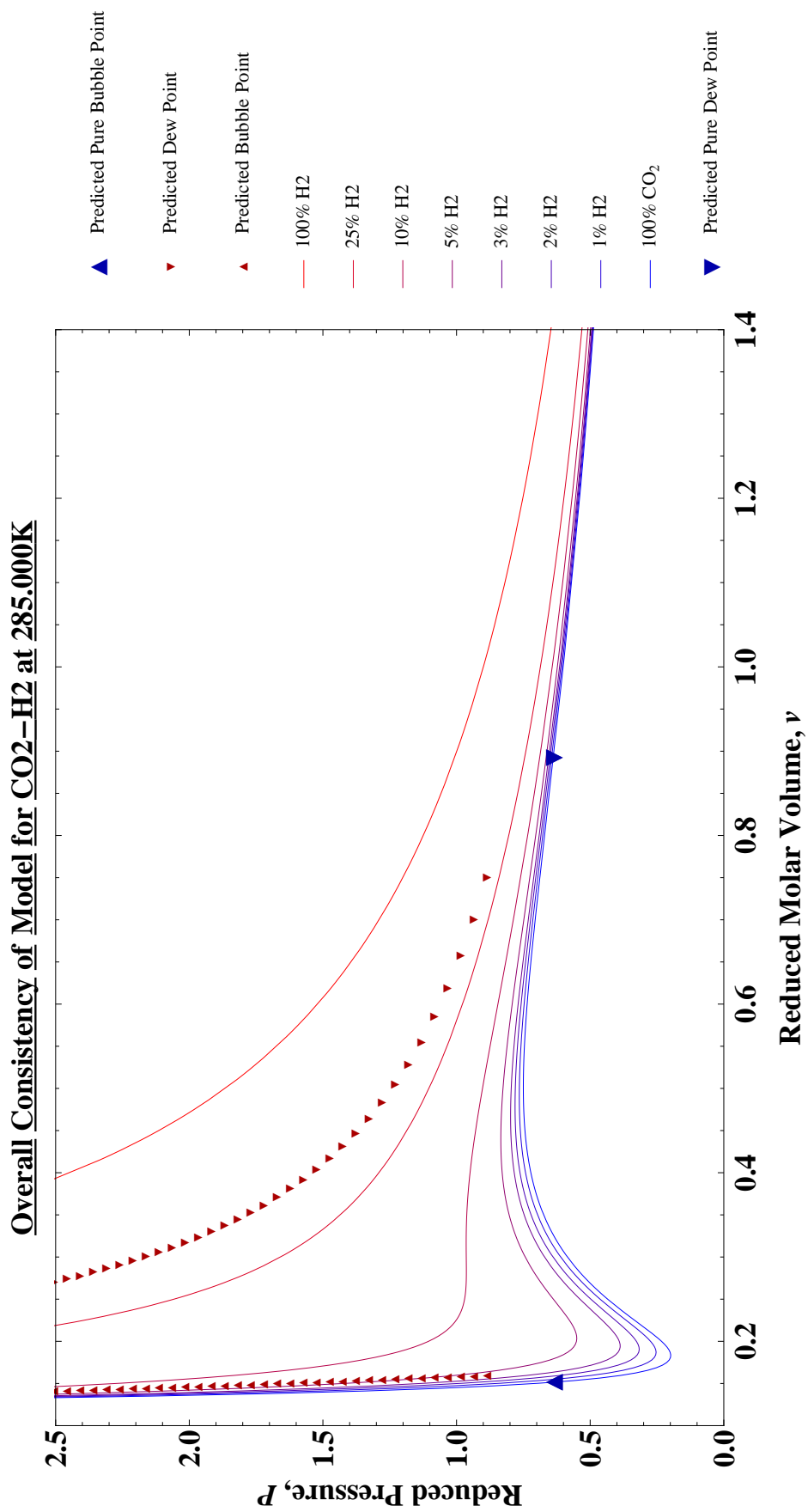


Figure 5.23: Pressure performance of model at 285K for carbon dioxide–hydrogen

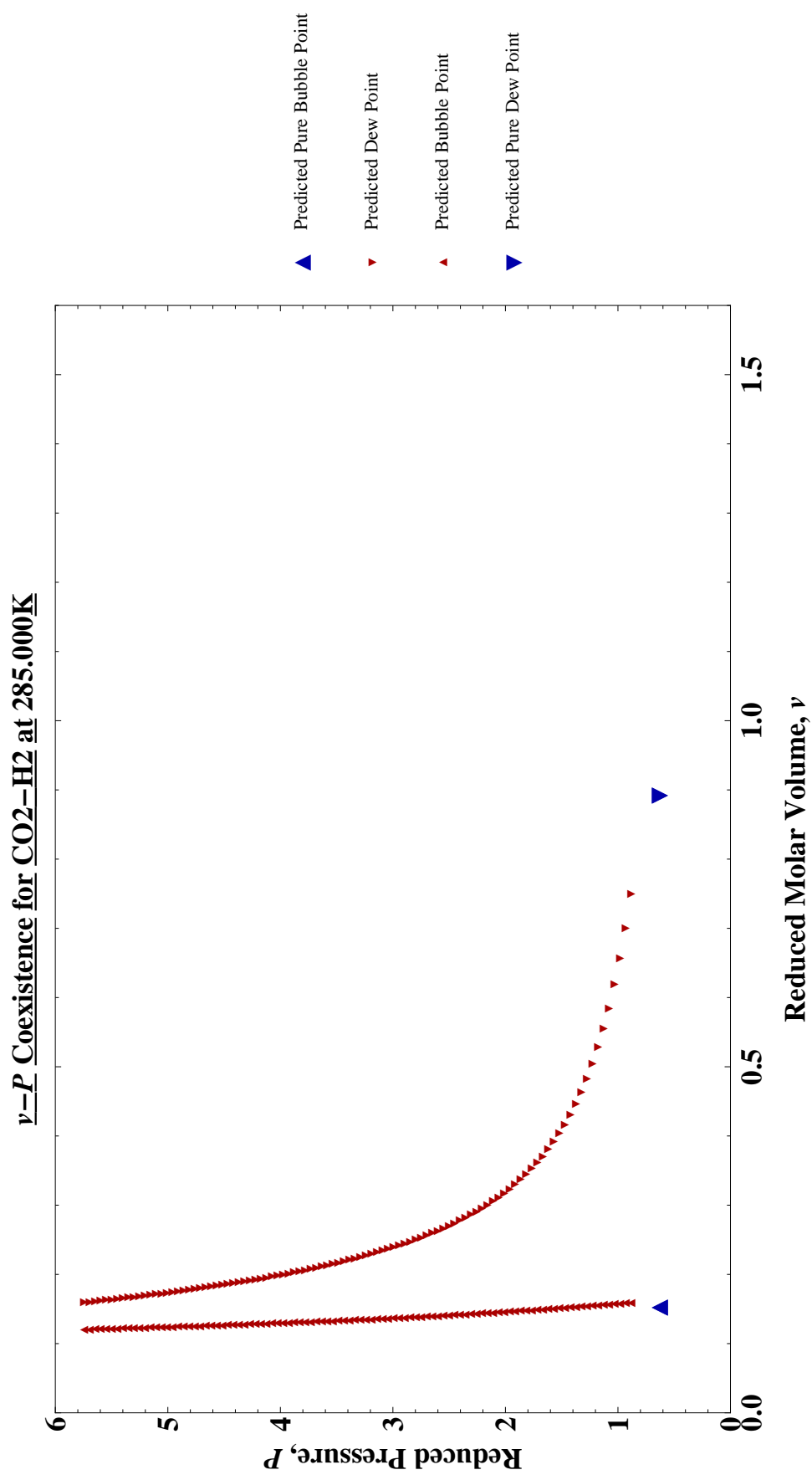


Figure 5.24: VLE coexisting volume performance of model at 285K for carbon dioxide-hydrogen

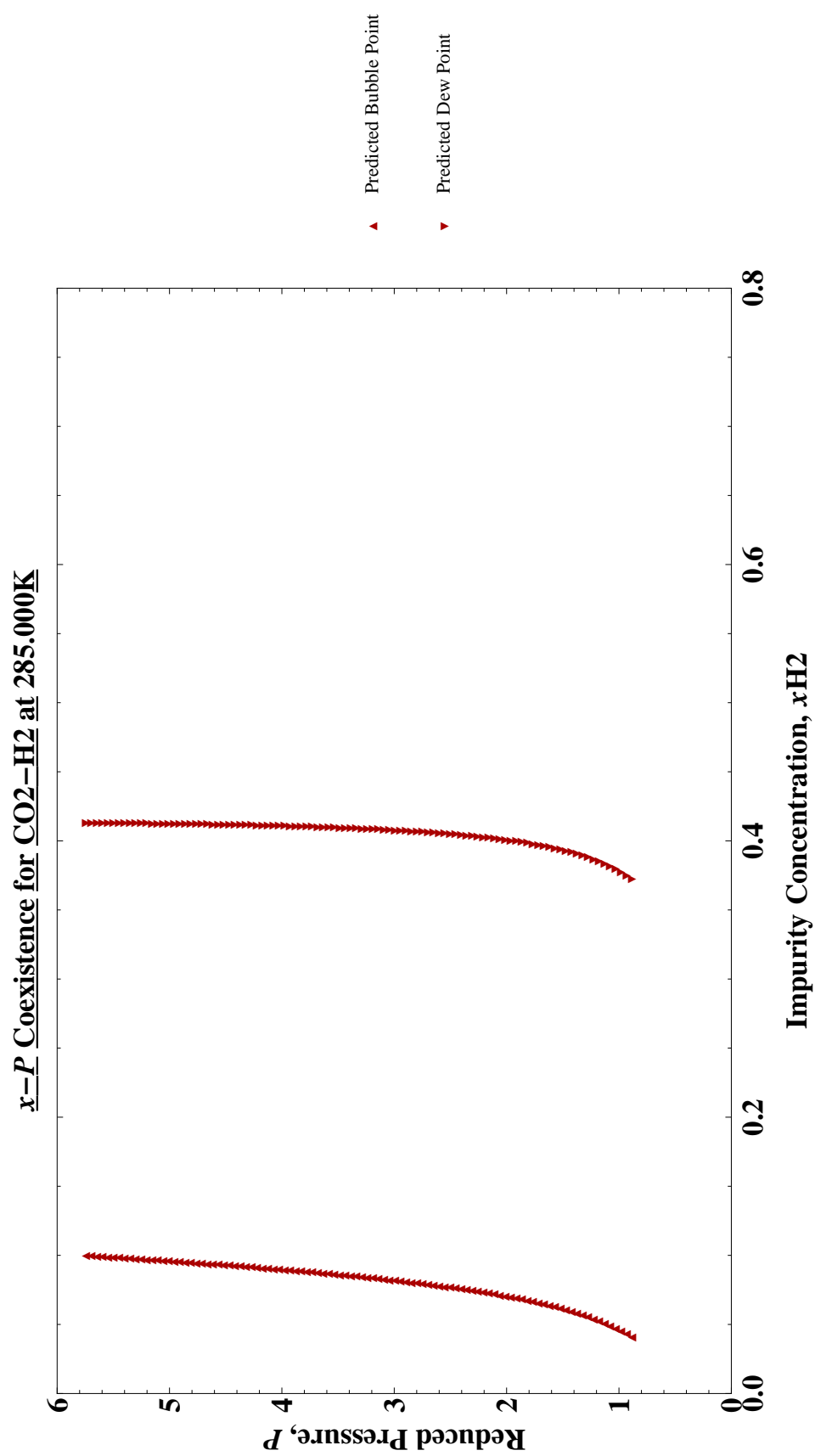


Figure 5.25: VLE coexisting mole fraction performance of model at 285K for carbon dioxide-hydrogen

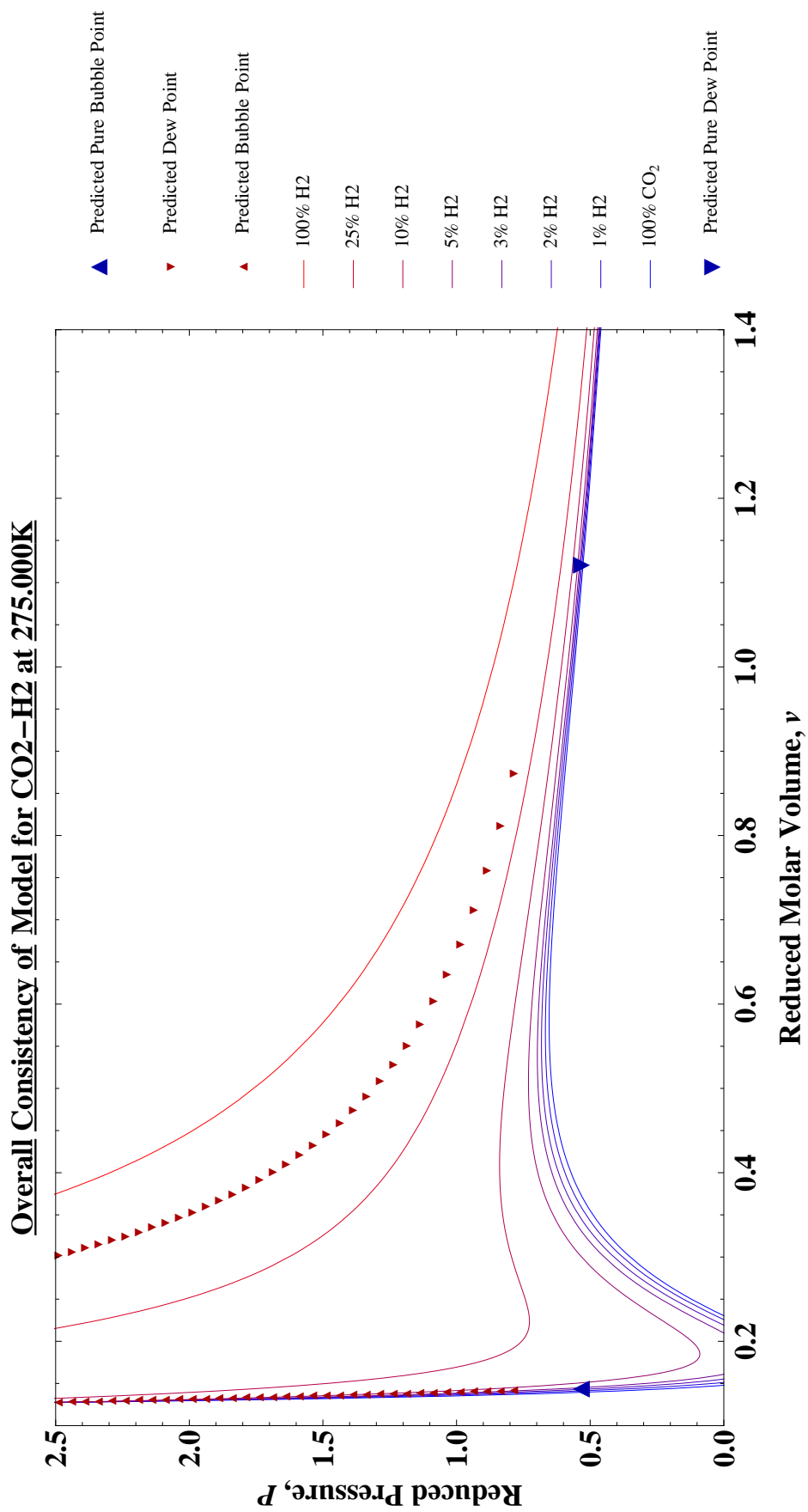


Figure 5.26: Pressure performance of model at 275K for carbon dioxide–hydrogen

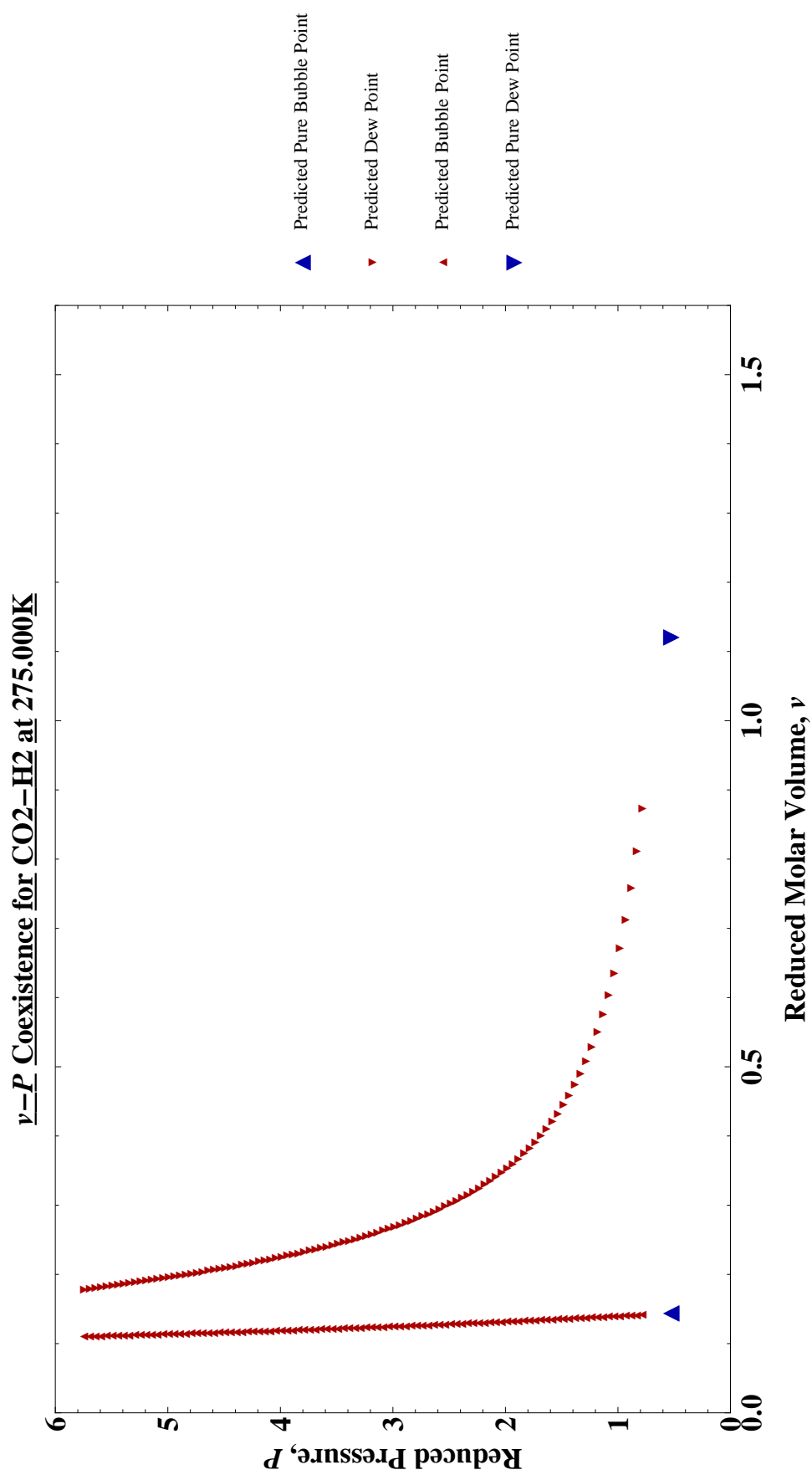


Figure 5.27: VLE coexisting volume performance of model at 275K for carbon dioxide-hydrogen

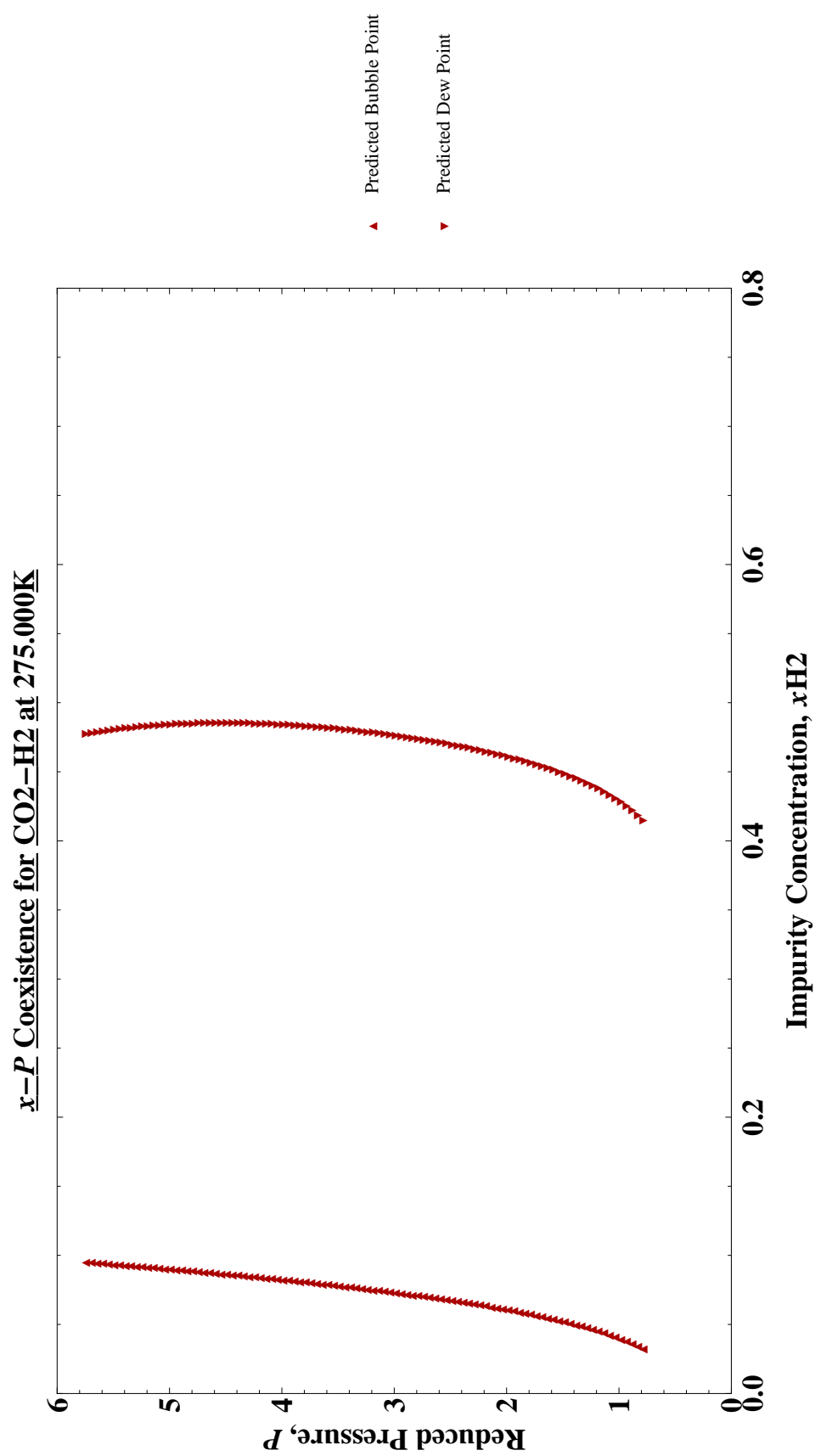


Figure 5.28: VLE coexisting mole fraction performance of model at 275K for carbon dioxide-hydrogen

These revealed a seemingly excellent behaviour, given the lack of literature data, right throughout the relevant range of temperatures. There did not appear to be any unphysical behaviour or contradictions, and the only issue we faced in generating and subsequently analysing these three plots was that at 295K we were unable to solve for the phase boundary, where we saw a lack of convergence at the top of the phase envelope. Nevertheless, in light of the performance of the other plots, we again felt confident that this showed the proposed equation to possess the potential to give good descriptions of the carbon dioxide–hydrogen system. Noting the difference in performance between the nitrogen binary system and the hydrogen binary system, we again attribute this to a lack of available data in the fitting stage which would constrain the VLE behaviour of the model.

5.5 Carbon Dioxide–Oxygen Binary Mixture

5.5.1 Data Availability

The situation with regard to availability of data in the carbon dioxide–oxygen system was found to be even more limited than for hydrogen, which was in turn more limited than for nitrogen. There was a single temperature at which the full array of VLE information was presented, at 273.15K (Muirbrook64 [54]), the highest temperature at which any VLE data was presented of 283.15K, and there was again no temperature at which both VLE and density data was given. A tabulated summary of the relevant available data is given in Table 5.15, again ordered by temperature.

| Temperature (K) | Homogeneous Density Data Sources | VLE Data Sources |
|---|----------------------------------|------------------------|
| 263.15 | | [112] † |
| 273.15 | | [112] †, [54], [103] † |
| 283.15 | | [112] † |
| 302.22 | [109] | |
| † means the VLE data in this source did not contain volumes | | |

Table 5.15: A summary of available data by source for carbon dioxide–oxygen binary mixtures

We can see from Table 5.15 that for the carbon dioxide–oxygen binary system there was just a single temperature point where the complete VLE data was given. Data was only presented at four temperature points in the range of interest, and again, we this created a scenario in which without the estimation techniques described in Chapter 2, we would have been unable to perform a single fitting (this again a key justification for our estimation methods). With these methods however, we were able to build the model around three temperature points: 283.15K, 273.15K, and 263.15K.

5.5.2 Fitting the Carbon Dioxide–Oxygen Binary Model Parameters

For fitting the carbon dioxide–oxygen parameters, we proceeded in exactly the same way as for fitting the nitrogen and then the hydrogen parameters, as discussed in Sections 5.3 and Section 5.4 respectively.

For finding the pure oxygen parameters we again set $W = 0.99$ in the error function for the pure oxygen parameters and for finding the binary interaction parameters for this system we set $W = 0.05$.

As a slight difference to how we proceeded before, owing to the smaller number of temperature points for this mixture, and the fact that most complete data set was available at 273.15K, we did the first step with simulated annealing at this temperature, then used local minimisation, taking the parameter values from this middle temperature, at the two other temperatures. The carbon dioxide–oxygen binary system parameters are summarised in Table 5.16.

| $T(\text{K})$ | a_{O_2} | b_{O_2} | c_{O_2} | d_{O_2} | e_{O_2} | f_{O_2} | g_{O_2} |
|---------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| 263.15 | 0.094921 | -0.208998 | -0.126906 | -0.132688 | -0.029934 | 0.723007 | 0.426078 |
| 273.15 | 0.124226 | -0.214169 | -0.042443 | -0.181688 | -0.094012 | 0.776980 | -0.494059 |
| 283.15 | 0.029317 | -0.205162 | -0.043949 | -0.136298 | -0.106251 | 0.447834 | -0.229049 |

| $T(\text{K})$ | $a_{\text{CO}_2,\text{O}_2}$ | $b_{\text{CO}_2,\text{O}_2}$ | $c_{\text{CO}_2,\text{O}_2}$ | $d_{\text{CO}_2,\text{O}_2}$ | $e_{\text{CO}_2,\text{O}_2}$ | $f_{\text{CO}_2,\text{O}_2}$ | $g_{\text{CO}_2,\text{O}_2}$ |
|---------------|------------------------------|------------------------------|------------------------------|------------------------------|------------------------------|------------------------------|------------------------------|
| 263.15 | 0.206934 | 0.463788 | 0.062166 | 0.685644 | -1.781140 | 0.624714 | -0.722116 |
| 273.15 | 0.188844 | 0.430426 | 0.151882 | 0.735649 | -1.031840 | 0.882312 | -0.445456 |
| 283.15 | 0.080006 | 0.554140 | 0.906305 | 0.639080 | -1.830015 | 0.143994 | 0.089705 |

Table 5.16: Fitted parameter values for the carbon dioxide–oxygen binary system

5.5.3 Preliminary Indications of Performance

After having found the fourteen parameters at each temperature point, we evaluated the performance of the proposed model to check the fitting that had been achieved through the optimisation of the error function had rendered a suitable representation of the data that was used to calibrate it in each case.

Just as for the two other binary mixtures, we did this by checking the percentage errors of the values suggested by our model for both the homogeneous density and VLE. A summary is in Table 5.17. We could see from this table that at 273.15K and 283.15K, an all round excellent performance was suggested, even though there was no homogeneous density data within the temperature range we considered. At 263.15K the performance was clearly a lot worse, and we again attribute this to a lack of sufficient data at this temperature.

| Temperature (K) | Homogeneous Density | | v_{BP} † | | v_{DP} † | | x_{O_2} † | | y_{O_2} † | |
|--|---------------------|---------|------------|---------|------------|---------|-------------|---------|-------------|---------|
| | Maximum | Average | Maximum | Average | Maximum | Average | Maximum | Average | Maximum | Average |
| 263.15 | 302.24 | 89.10 | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |
| 273.15 | 11.19 | 2.43 | 5.82 | 3.03 | 34.43 | 15.76 | 8.37 | 4.27 | 34.69 | 21.26 |
| 283.15 | 13.28 | 3.80 | 7.48 | 3.88 | 34.45 | 17.53 | 5.63 | 2.81 | 20.23 | 9.60 |
| † where convergence to a meaningful solution had been possible | | | | | | | | | | |

Table 5.17: Preliminary testing of predictions made by our model for the carbon dioxide–oxygen binary system

5.5.4 Variation of Model Parameters with Temperature

We again specified a quadratic temperature dependence for each parameter in the carbon dioxide–oxygen system, as for the binary mixtures involving nitrogen and hydrogen. We carried out the same procedure as before to determine these dependences, and obtained the following:

$$a_{O_2}(T) = -45.3188 + 102.191T - 57.4457T^2 \quad (5.74)$$

$$b_{O_2}(T) = 5.0224 - 11.7192T + 6.55663T^2 \quad (5.75)$$

$$c_{O_2}(T) = -33.2466 + 72.6782T - 39.7581T^2 \quad (5.76)$$

$$d_{O_2}(T) = 35.0799 - 78.4664T + 43.6521T^2 \quad (5.77)$$

$$e_{O_2}(T) = 20.2866 - 44.2235T + 23.9734T^2 \quad (5.78)$$

$$f_{O_2}(T) = -138.389 + 314.082T - 177.181T^2 \quad (5.79)$$

$$g_{O_2}(T) = 121.039 - 273.628T + 153.998T^2 \quad (5.80)$$

$$a_{CO_2,O_2}(T) = -31.9314 + 73.4563T - 41.968T^2 \quad (5.81)$$

$$b_{CO_2,O_2}(T) = 57.7945 - 129.114T + 72.6431T^2 \quad (5.82)$$

$$c_{CO_2,O_2}(T) = 236.595 - 539.354T + 307.407T^2 \quad (5.83)$$

$$d_{CO_2,O_2}(T) = -53.3081 + 121.054T - 67.7856T^2 \quad (5.84)$$

$$e_{CO_2,O_2}(T) = -577.655 + 1284.78T - 715.657T^2 \quad (5.85)$$

$$f_{CO_2,O_2}(T) = -364.083 + 820.022T - 460.581T^2 \quad (5.86)$$

$$g_{CO_2,O_2}(T) = 84.9019 - 202.398T + 119.549T^2 \quad (5.87)$$

We can see from Figures 5.29 and 5.30 how these temperature dependences resembled the parameter values at the chosen temperature points.

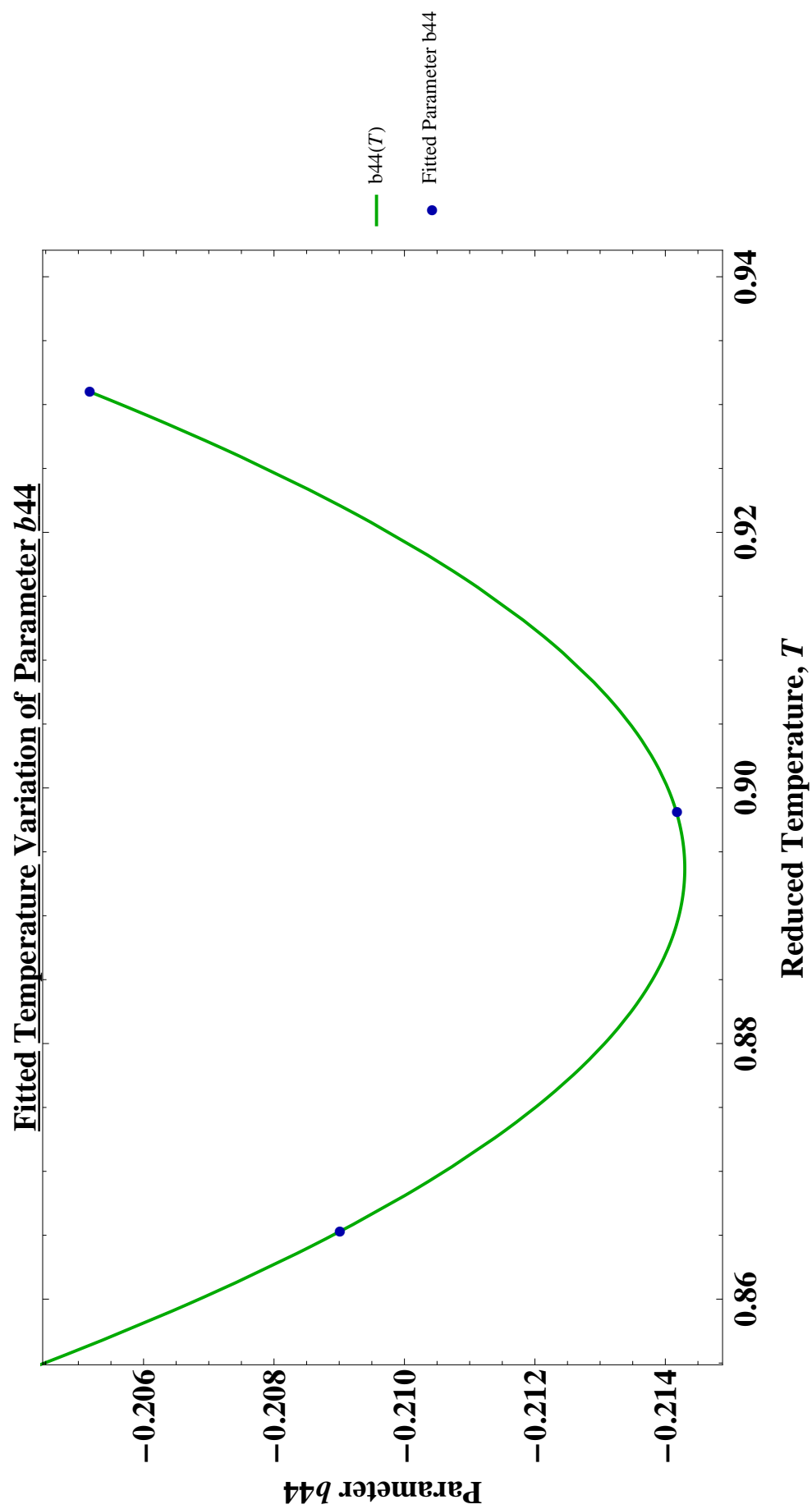


Figure 5.29: Temperature dependence for the pure oxygen parameter b_{O_2} (denoted in the graph by b_{44})

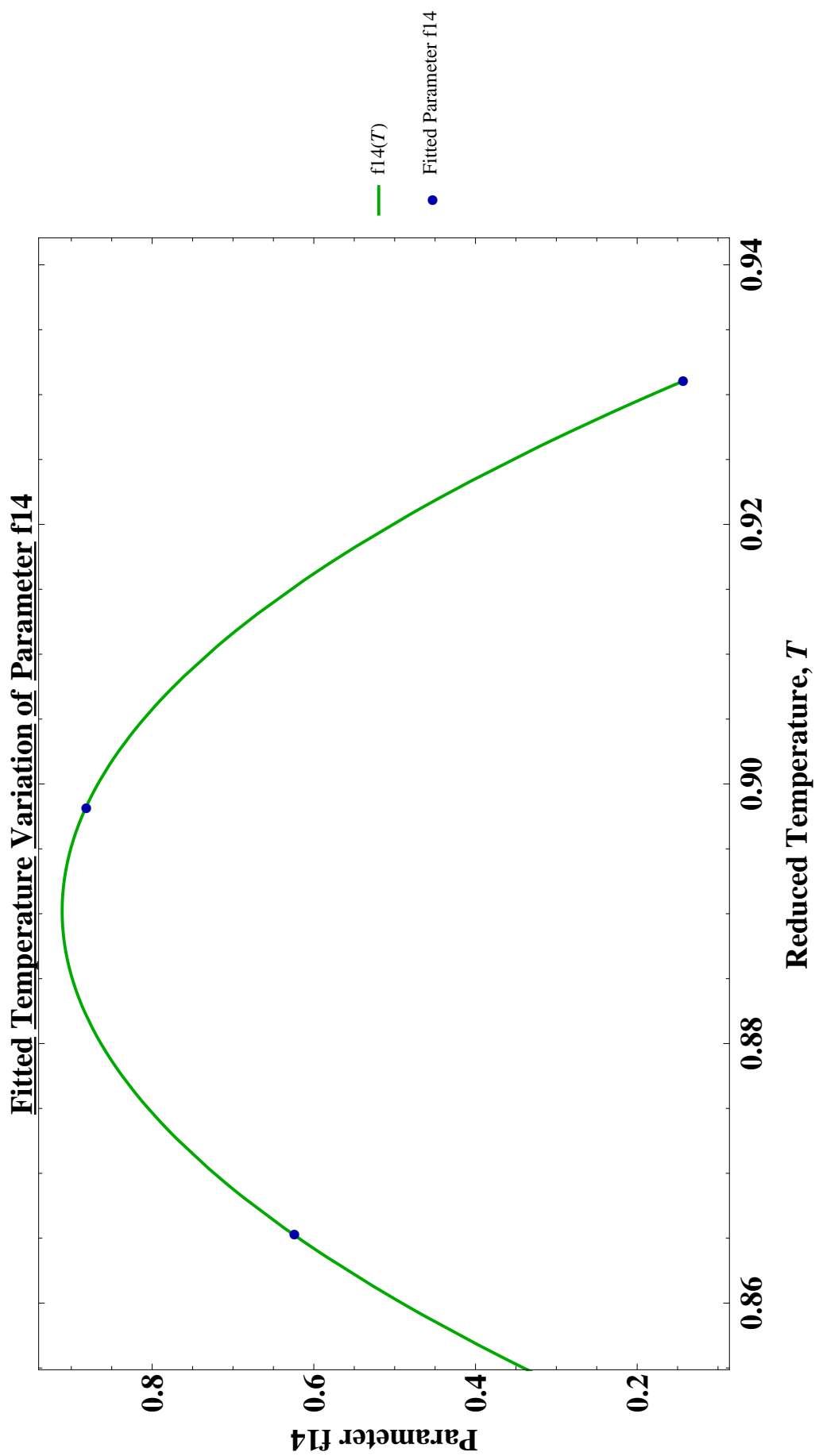


Figure 5.30: Temperature dependence for the binary interaction parameter $f_{\text{CO}_2, \text{O}_2}$ (denoted in the graph by f_{14})

5.5.5 Performance of the Full Model for Binary Mixtures of Carbon Dioxide and Oxygen

This closed the model for the binary system involving carbon dioxide and oxygen, and with it, all three binary systems we sought to describe. Using this full definition, we were able to assess the performance of the final model for this case. We did this by once again comparing the model at temperature points which had been used to generate the fitted parameters, and then by checking the performance at temperatures where no data existed in order to check performance there. We note that since we fit the model parameters between 263.15K and 283.15K, we would not expect meaningful descriptions to be given significantly outside this range, in particular approaching the carbon dioxide critical temperature.

We began by comparing the behaviour of our model to the homogeneous volume–pressure data at 283.15K:

| Oxygen Composition (%) | Maximum Error (%) | Average Error (%) |
|------------------------|-------------------|-------------------|
| 2.8 (liquid phase) | 13.28 | 3.27 |
| 4 (liquid phase) | 9.06 | 3.77 |
| 7.1 (liquid phase) | 11.19 | 8.47 |
| 11.5 (vapour phase) | 3.91 | 0.74 |
| 16.1 (vapour phase) | 5.37 | 1.27 |
| 21.8 (vapour phase) | 6.99 | 1.96 |
| 100 | 3.36 | 1.81 |
| ALL | 13.28 | 3.80 |

Table 5.18: Pressure performance of the model at 283.15K

We also compared the behaviour of our model to the VLE data at 283.15K:

| Quantity | Maximum Error (%) | Average Error (%) |
|--|-------------------|-------------------|
| v_{BP} † | 6.23 | 3.42 |
| v_{DP} † | 68.75 | 37.50 |
| x_{O_2} † | 10.72 | 5.59 |
| y_{O_2} † | 28.25 | 16.86 |
| ALL | 68.75 | 15.88 |
| † where convergence to a meaningful solution had been possible | | |

Table 5.19: VLE performance of the model at 283.15K

We note that, as was the case for both nitrogen and hydrogen, most predictions were around our target accuracy range, with the exception of the bubble curve volumes, demonstrating once more that the model possessed sufficient flexibility to be able to also model this binary system with sufficient accuracy for the needs of CCS pipeline operators. Once again we highlight the best performance of our model as occurring at the liquid saturation line. Overall, we felt the behaviour of the model exhibited at this temperature was excellent in light of the fact that there had been no homogeneous density or coexisting volume data here, giving further credibility

to our homogeneous density estimation methods. We can again verify in Figures 5.31 to 5.33 that the behaviour of our model was broadly consistent with the data.

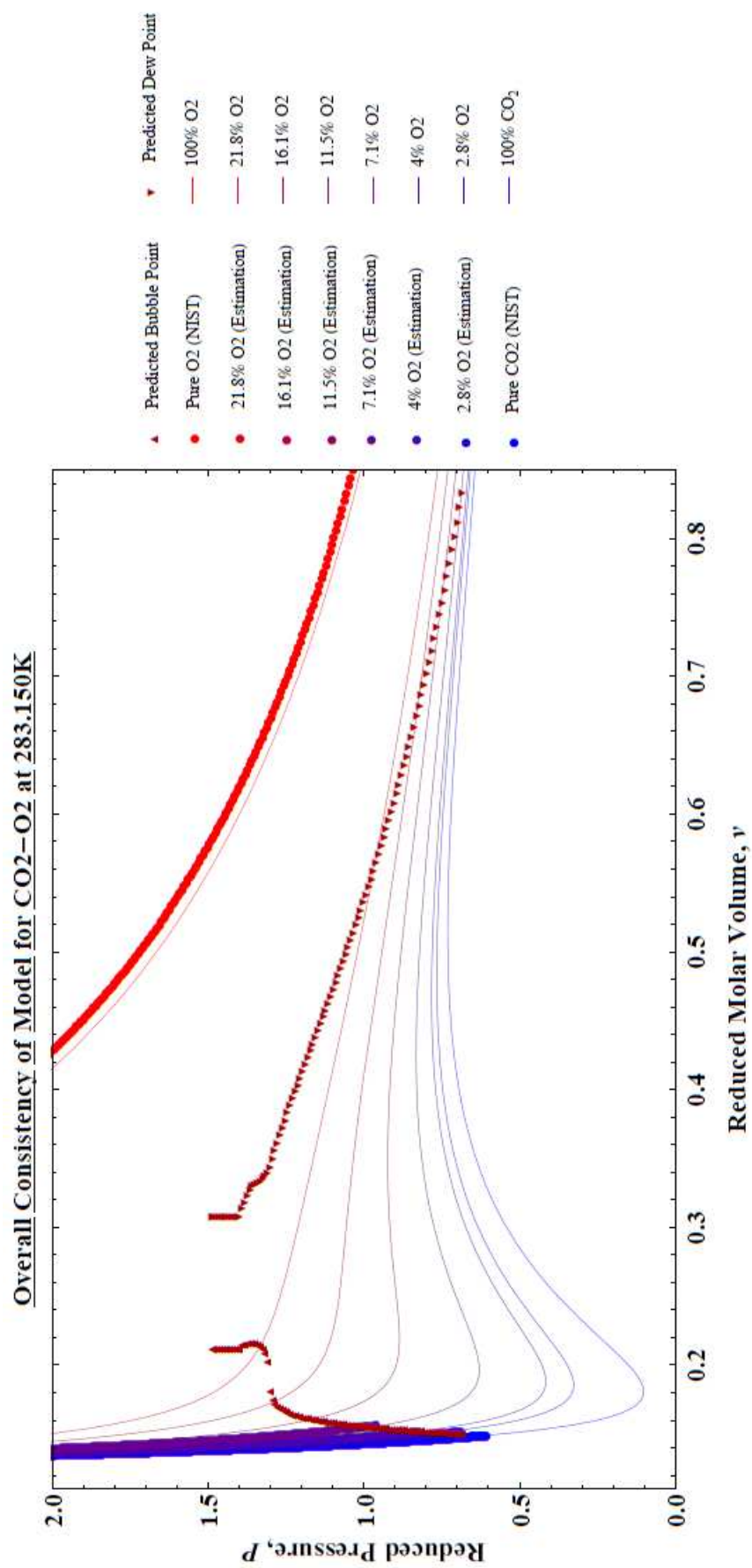


Figure 5.31: Pressure performance of model at 283.15K for carbon dioxide-oxygen

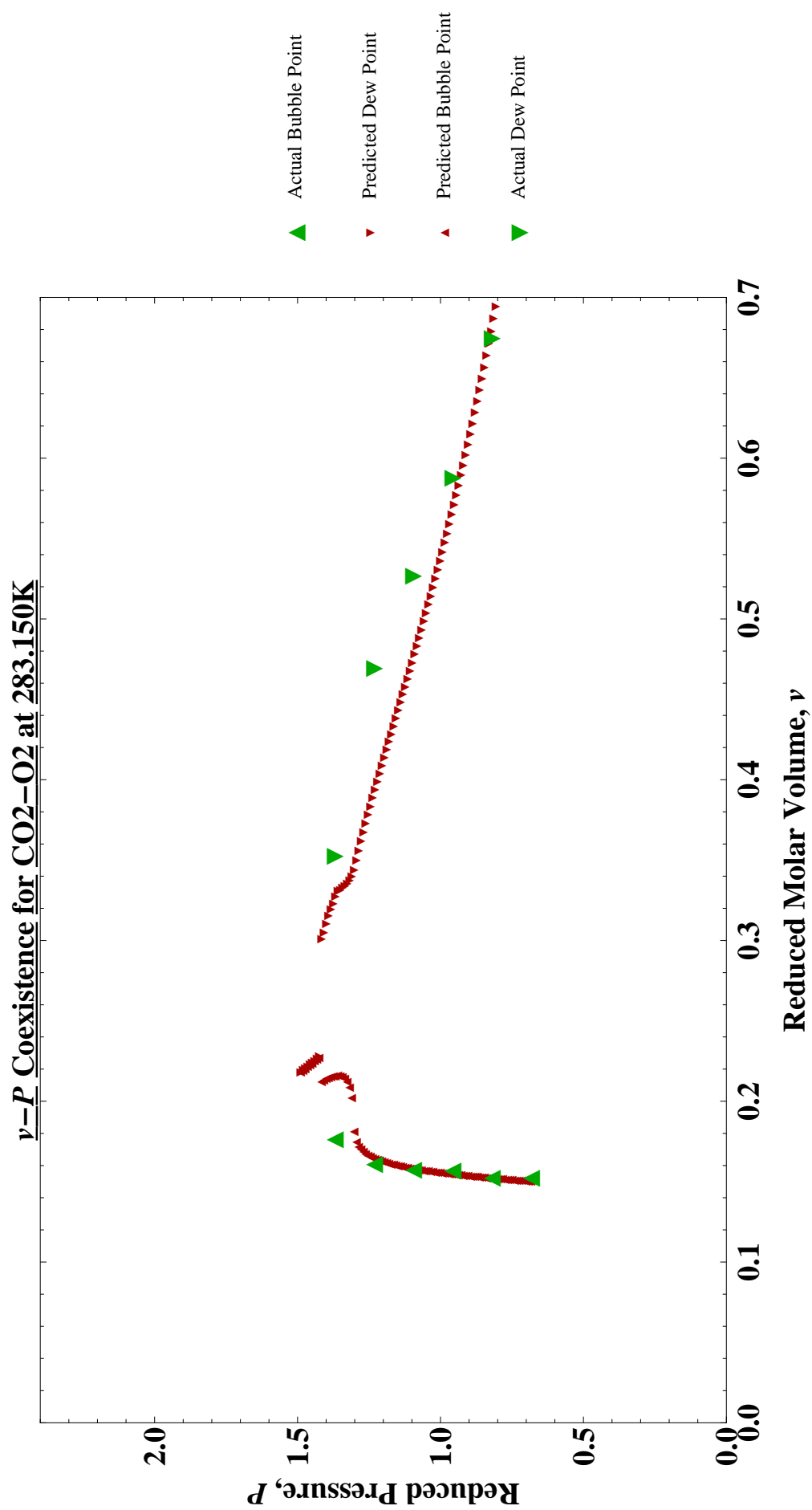


Figure 5.32: VLE coexisting volume performance of model at 283.15K for carbon dioxide-oxygen

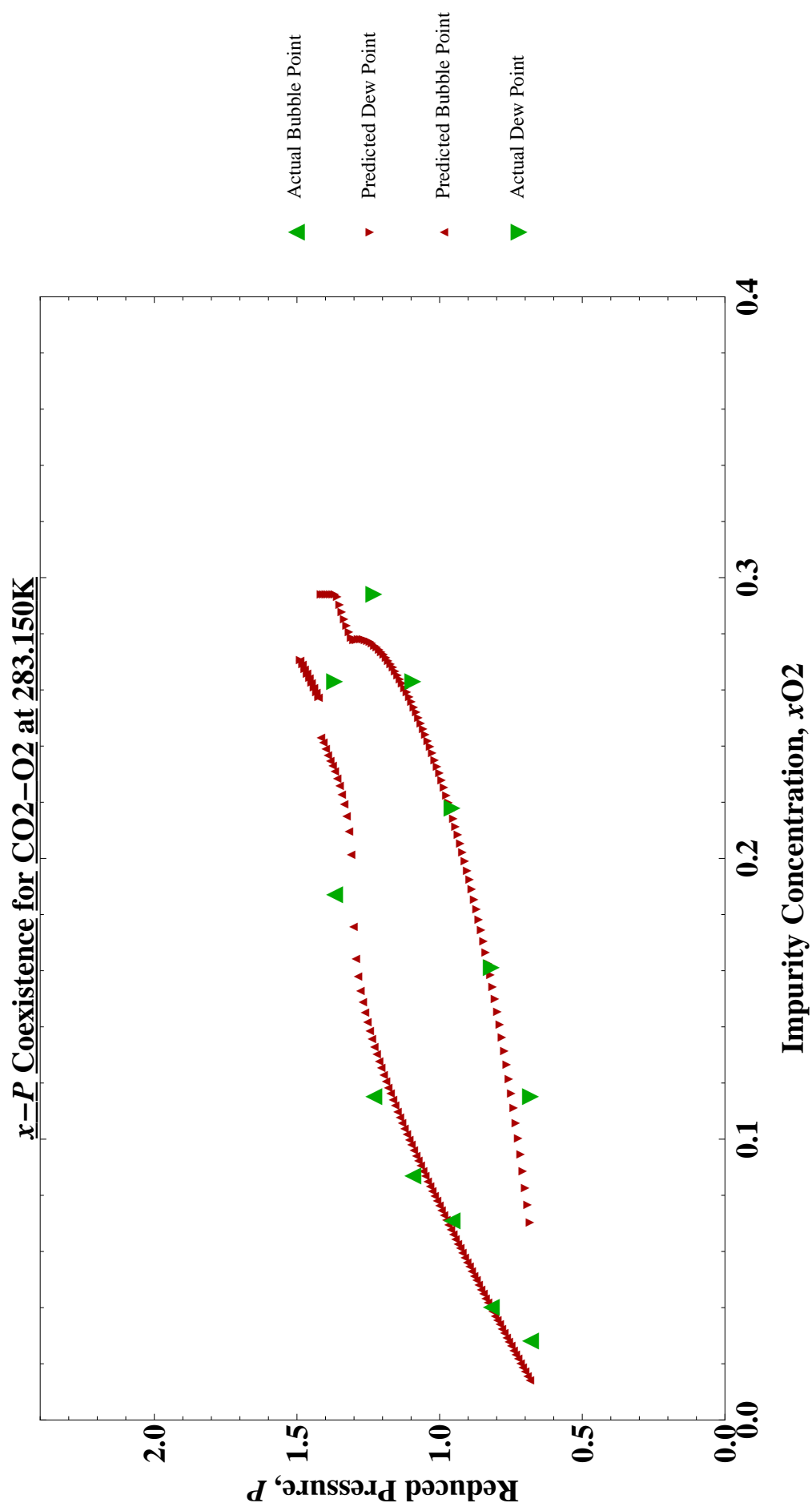


Figure 5.33: VLE coexisting mole fraction performance of model at 283.15K for carbon dioxide–oxygen

We then compared the behaviour of our model to the homogeneous volume–pressure data at 273.15K:

| Nitrogen Composition | Maximum Error (%) | Average Error (%) |
|----------------------|-------------------|-------------------|
| 0.66 (liquid phase) | 11.19 | 2.42 |
| 1.41 (liquid phase) | 3.57 | 1.38 |
| 2.18 (liquid phase) | 4.51 | 2.60 |
| 4.8 (vapour phase) | 1.27 | 0.29 |
| 9.9 (vapour phase) | 2.55 | 0.57 |
| 14.5 (vapour phase) | 3.58 | 0.98 |
| 100 | 8.71 | 3.80 |
| ALL | 11.19 | 2.43 |

Table 5.20: Pressure performance of the model at 273.15K

We also compared the behaviour of our model to the VLE data at 273.15K:

| Quantity | Maximum Error (%) | Average Error (%) |
|--|-------------------|-------------------|
| v_{BP} † | 5.12 | 1.95 |
| v_{DP} † | 85.02 | 40.35 |
| x_{N_2} † | 9.20 | 3.88 |
| y_{N_2} † | 29.22 | 18.12 |
| ALL | 85.02 | 16.08 |
| † where convergence to a meaningful solution had been possible | | |

Table 5.21: VLE performance of the model at 273.15K

The performance of the model at both these temperatures was again seen to be excellent. Here in particular, we can clearly see the effect of having had high quality literature data such as the VLE measurements which were available at 273.15K in [54]. Such data allowed us to achieve a very good fitting and to produce a model which is extremely faithful to the real behaviour of this binary system, often displaying errors under 1% (see Table 5.20). We checked the behaviour of the model at this temperature for consistency in Figures 5.34 to 5.36, and again saw that at low concentrations of oxygen impurity, as can be expected in CCS pipelines [31], an excellent description is given. Following on from this analysis, we generated one final plot at 275K in order to ensure consistent and physical behaviour at other temperatures.

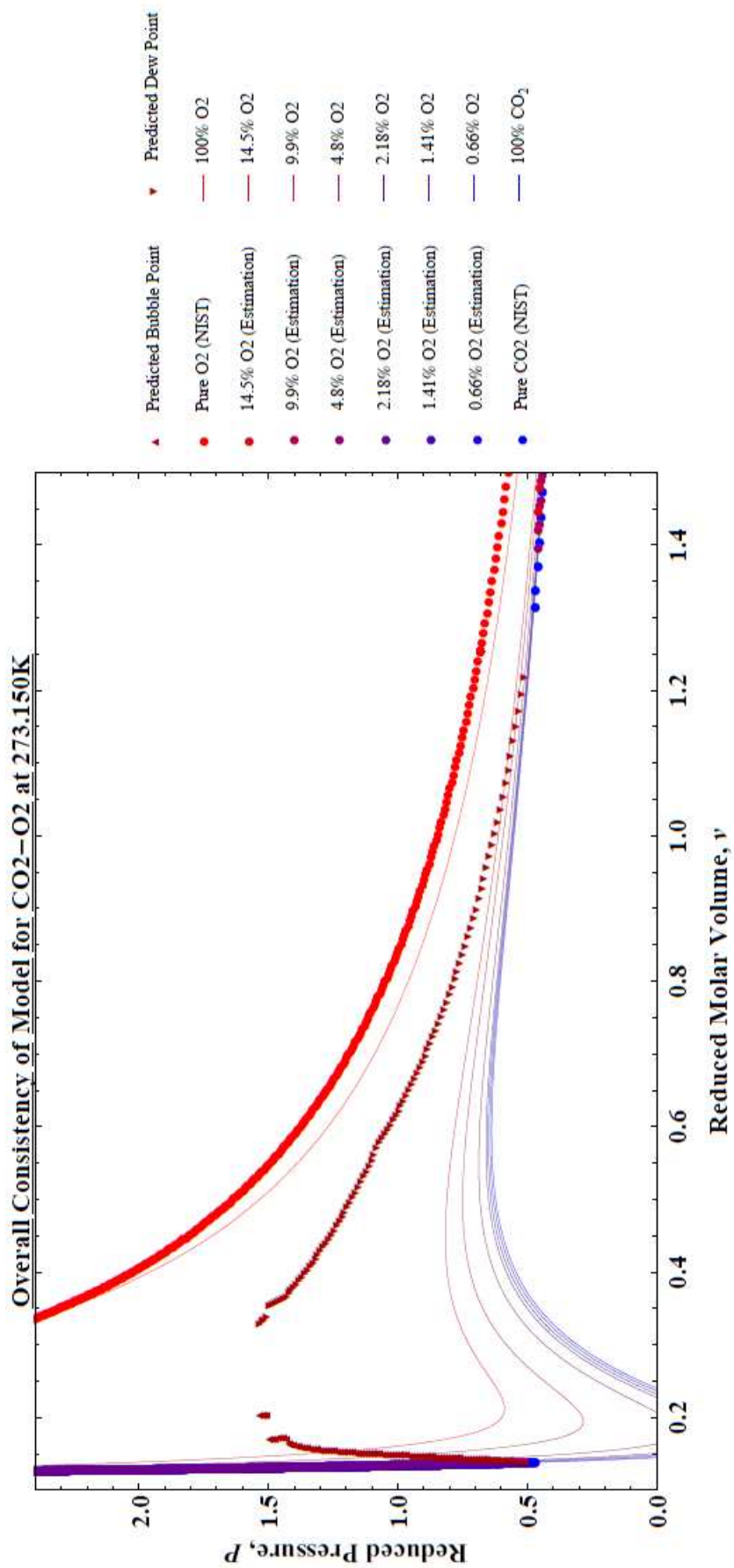


Figure 5.34: Pressure performance of model at 273.15K for carbon dioxide-oxygen

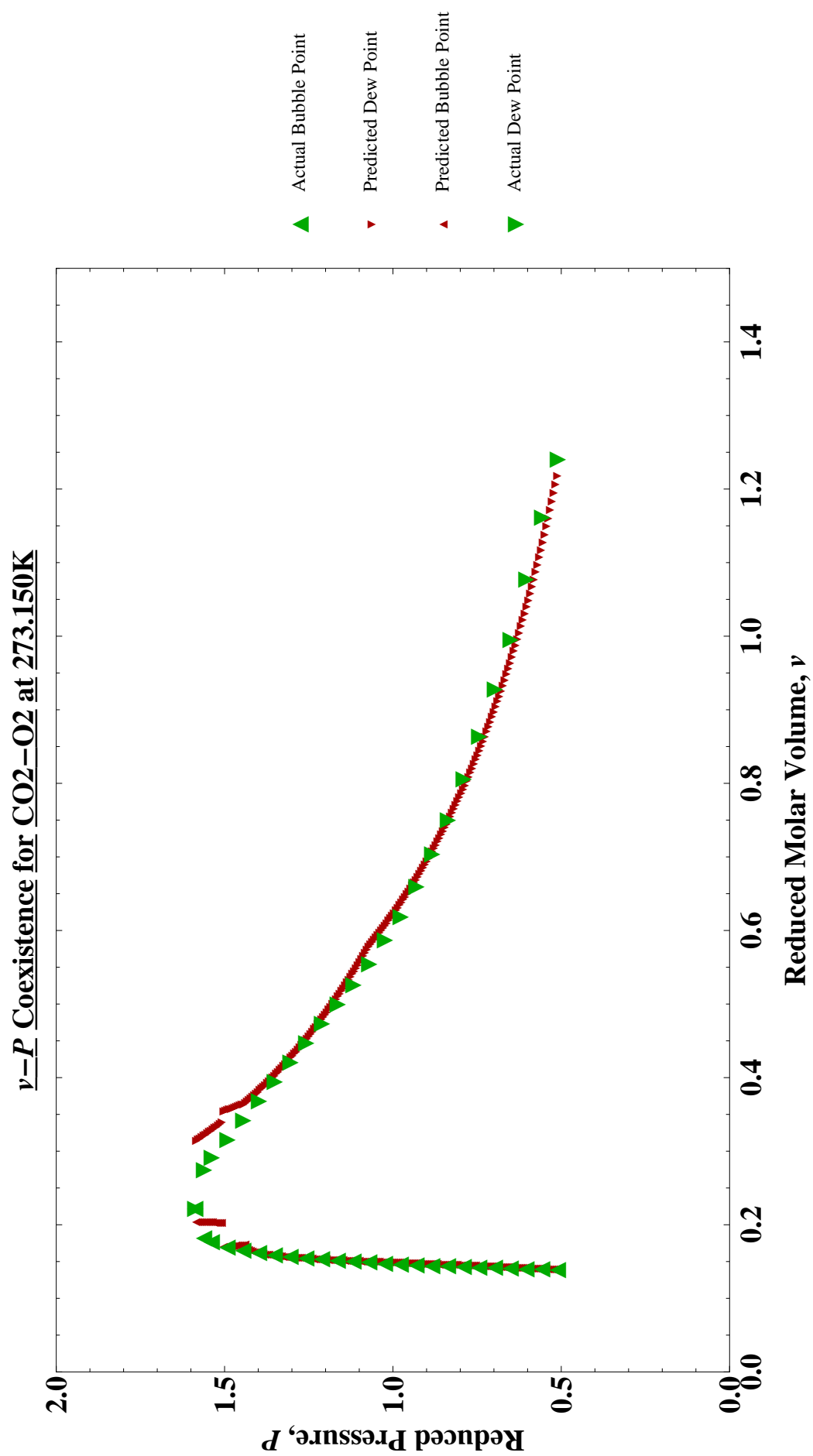


Figure 5.35: VLE coexisting volume performance of model at 273.15K for carbon dioxide–oxygen where a comprehensive data set was available

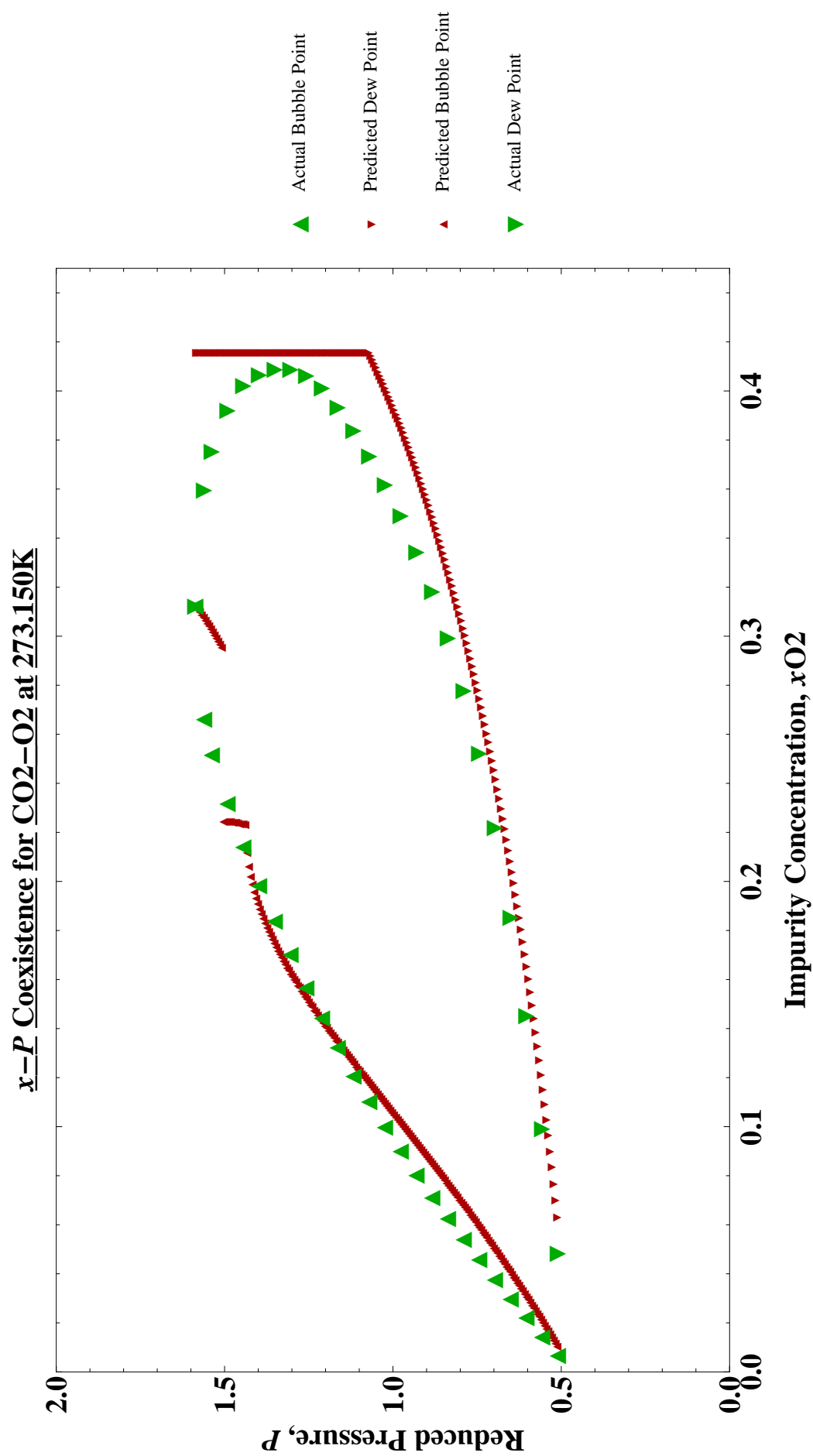


Figure 5.36: VLE coexisting mole fraction performance of model at 273.15K for carbon dioxide-oxygen

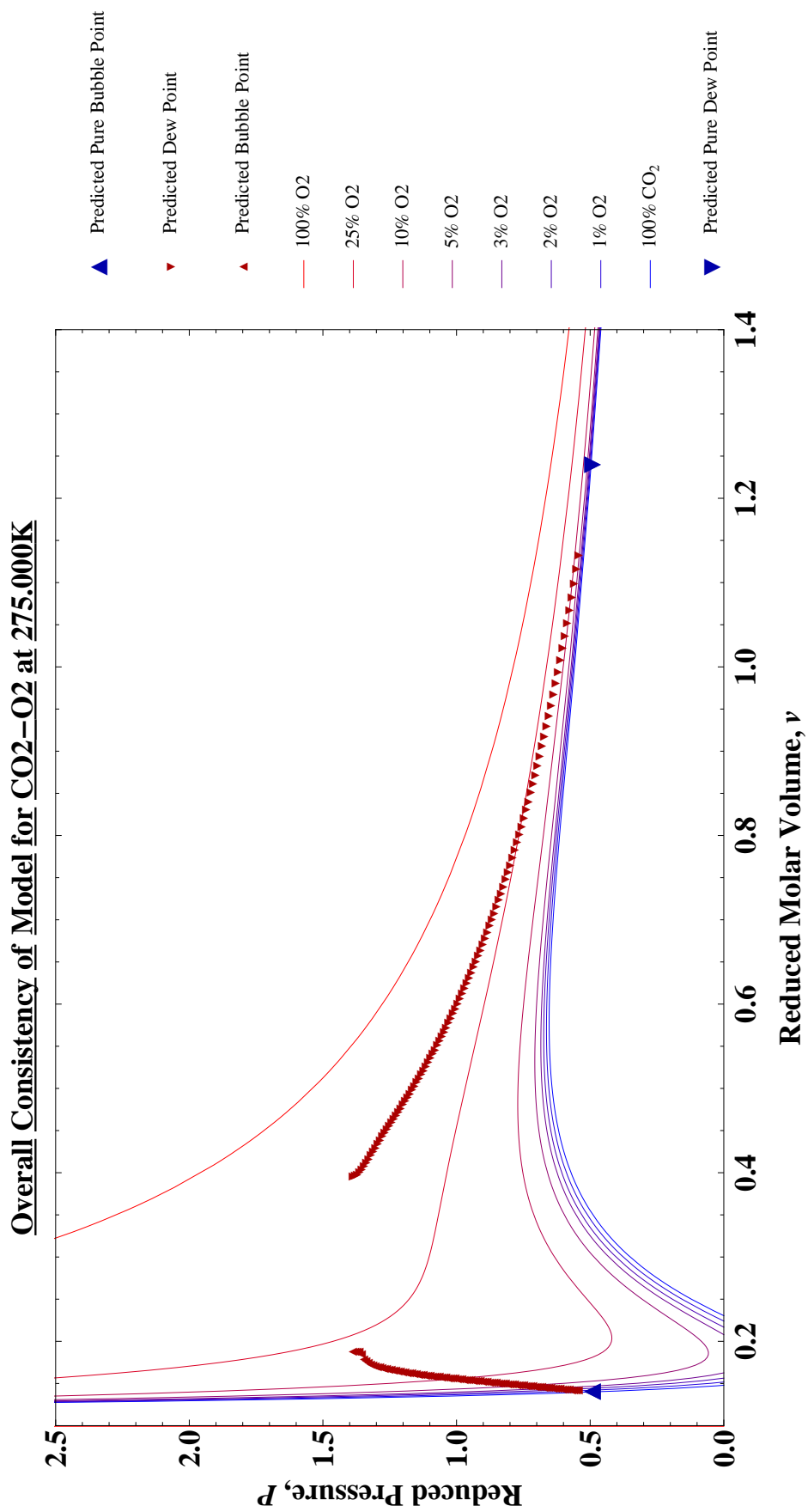


Figure 5.37: Pressure performance of model at 275K for carbon dioxide-oxygen

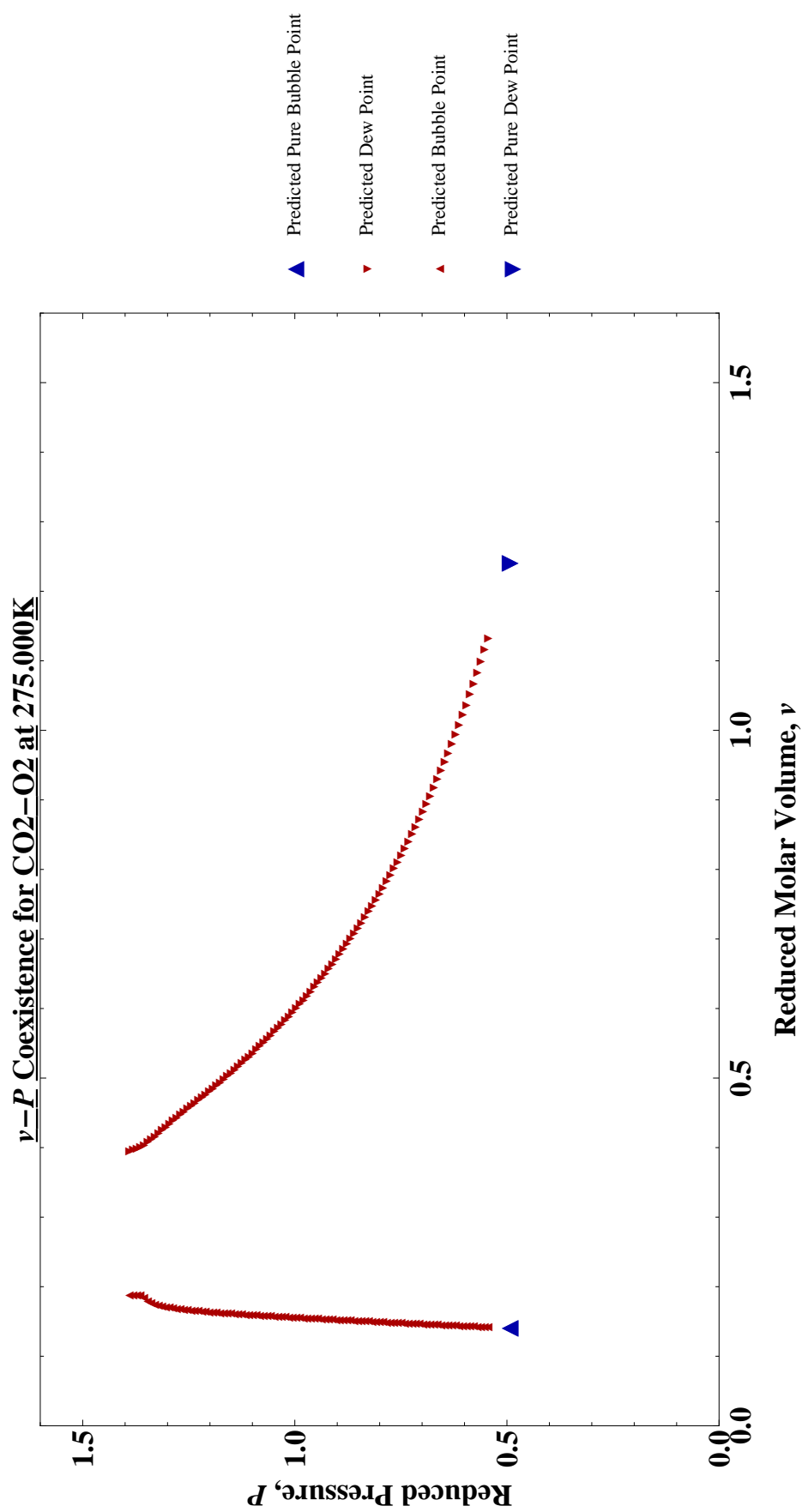


Figure 5.38: VLE coexisting volume performance of model at 275K for carbon dioxide–oxygen

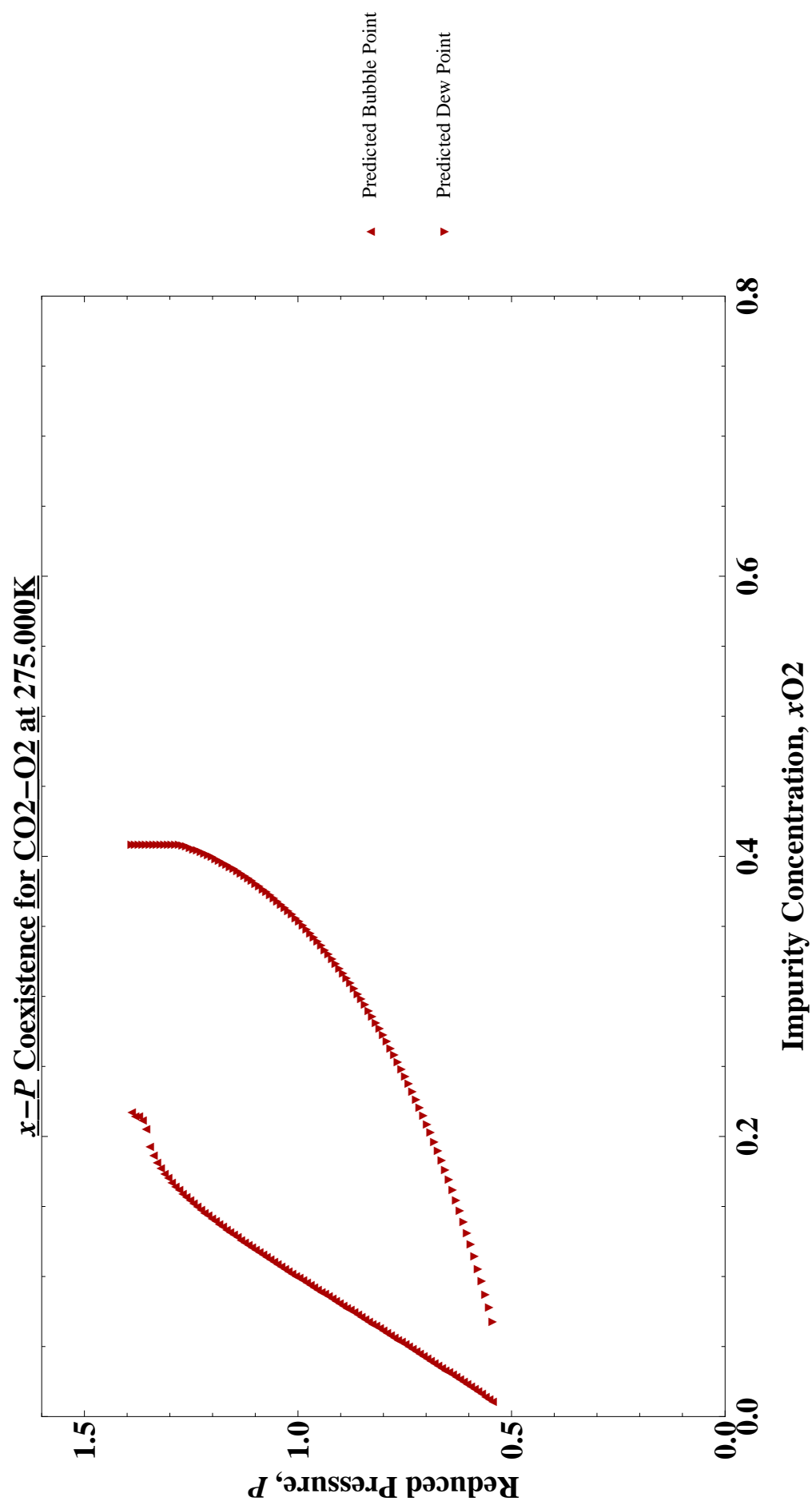


Figure 5.39: VLE coexisting mole fraction performance of model at 275K for carbon dioxide-oxygen

Considering the very limited amount of data we had access to in fitting the carbon dioxide–oxygen model, we felt the performance was again excellent and was further demonstration of the ability of our EoS to predict physical behaviour with a high accuracy. Where the predictions for this mixture were been found to be lacking, specifically in Figures 5.33 and 5.36 where the root finding algorithm for solving to find the VLE fails at some points, we can again attribute this to the lack of middle composition density data which is required to constrain the VLE behaviour close to the critical point. Nevertheless, this capped an excellent performance of our model in reconstructing the binary system of carbon dioxide and oxygen.

Chapter 6

Conclusions and Further Work

6.1 Overview

We set out on this project aiming to develop a new equation of state for use in the design and operation of CCS transport pipelines, which could be relied upon to not be more than 2% out in giving any homogeneous phase density or vapour–liquid equilibrium predictions. Following on from an extensive contextual literature review, we had established that there were many reasons why this was required; principal among them the pressing need for a formulation that would allow users to ensure the pipelines were both safe and cost-effective.

We identified and developed a mathematical method that could be used to calibrate a model which we proposed as part of this work. To allow us to calibrate this proposal into a meaningful equation of state, we began by harvesting a wealth of data for mixtures including homogeneous density and coexistence data from various literature sources and the NIST website.

In the case of pure carbon dioxide we found that the combination of our proposed formulation in Equation (3.9) and the method we had specified in Chapter 2 was able to capture the physical data to a very high degree of accuracy. We had a paper on this part of the work published [40] and in this thesis offered an update that was a slight improvement on this, in terms of accuracy, consistency of behaviour, and of range of validity.

In moving forward to incorporating mixtures to the model we also developed a

formulation relating the fugacity of a substance in a mixture with that of the same substance when in pure form. This allowed us to far more conveniently ensure the correct phase behaviour in fitting the binary data.

There were a number of key outputs from this work:

Firstly, in Equation (3.9) we proposed the formulation for a model which exhibited a high degree of accuracy in describing physical behaviours in the cases where data existed for us to use in fitting the model. We demonstrated the accuracy of our model over the full range of CCS pipeline relevant temperatures and pressures for pure carbon dioxide, as well as in a more limited temperature range in the carbon dioxide–nitrogen binary system, where predictions were seen to be well within the target range. The model also proved extremely useful in reconstructing with great accuracy the behaviour at individual temperature points in the binary systems carbon dioxide–hydrogen and carbon dioxide–oxygen, where a relative lack of data for fitting meant that the same broad accuracy as in the nitrogen case could not be reached, although the predictions still fell broadly within or very close to the target we set. We feel confident that the proposed model could therefore be used throughout the whole range of relevance, if sufficient characterising thermodynamic data were available, specifically middle composition (40-60%) supercritical homogeneous density data, which would constrain the VLE behaviour of the model all the way to the critical point for that mixture at the relevant temperature.

Secondly, we developed a method by which the equation sought in our original aims could be calibrated and developed. Specifically; given a proposed equation in the form $P(v)$ and supplementary mixing rules, we developed a method to obtain all the required fugacity expressions and to fit the model parameters to that data which was available. We utilised this method to fit the proposed model in a range of conditions as allowed by the data we had collected, and we feel confident that once calibrated, our model had the ability to exhibit some very reasonable accuracy. Where suitable data had been available to affect a meaningful fitting, we generally found our models to exhibit errors ranging from 0 to 3% for the two different types of physical predictions.

Thirdly, by way of addressing some of the limitations of the VLE data, we developed a novel method of estimating the molar volumes at the phase boundary where such information had not been reported. We demonstrated the accuracy and suitability of these methods as part of this thesis.

Fourthly, having conducted what we believe to be a thorough review of the thermodynamic data available within the literature, and employed this in the fitting of our model, we are absolutely clear in the reason why we were ultimately unable to finalise the EoS over the whole temperature range. This was because of a lack of sufficient data in the literature which the model could be calibrated to. Specifically, we found that there was an almost total lack of any cases of homogeneous density data being given at the same temperature as VLE data. Furthermore, the majority of the VLE data did not quote the full thermodynamic description, often missing coexisting molar volumes, and so we were not, without some extra insight, able to provide a fitting which simultaneously rendered a useful description of both density and coexistence conditions. Furthermore, we were able, as part of the conclusions of this work, to identify the thermodynamic data which was missing from the literature, and in doing so specify precisely which measurements need to be taken by the CCS community at large in order for our method of calibration to be used. These are highlighted in Section 6.5. If this would be possible, then based on the success of our model and method where data had been available, we felt the aims could be achieved in their entirety.

We have established an effective framework for deriving a new equation of state, calibrating a proposed form to literature data. Our work opens up many new avenues for future research.

6.2 Key Results and Outputs

Chapter 2 highlighted the key physical constraints that needed to be enforced if physically correct behaviour was to be predicted by the model. We specified these for both VLE coexistence conditions, which were imposed at the boundary of the two-phase region, and for the homogeneous density, which were imposed away from the two-phase region in the homogeneous phase. This was in the form of an error function which we could seek to minimise by use of the simulated annealing and local root finding routines programmed in the Mathematica software. We also performed nondimensionalisations of these so that when a nondimensional EoS was presented, these routines could search more easily through the parameter space.

We outlined the features the data had to possess in order to be of any use to us in fitting, and subsequently noted that much of the VLE data presented in the literature was missing a volumetric element at coexistence. In order to compensate for this, we developed a novel method of estimating these values, based on weighted

averages of molar volumes of the carbon dioxide and the second component of the binary mixture being considered. Our methods of volume estimation later proved invaluable in fitting binary mixtures in each of the three cases we worked with.

Chapter 3 saw a proposal of a new, seven-parameter equation of state for use in determining the physical properties of pure CO₂ in the case of pipeline transport for CCS. This would lay the foundation to allow us extend the model into descriptions of the mixture behaviour, as well as to allow us to easily to extend the range of temperatures and pressures if this was deemed necessary. Given our aim of finding an equation which exhibited accuracy superior to the Peng–Robinson Equation of State [34] without necessitating a significant additional functional complexity, we were immediately able to verify that our equation was comparable to the PREoS in terms of complexity, as required. We motivated the form of our equation to allow the reader to confirm that it would render a sufficient flexibility to model the data whilst retaining a faithfulness to the broad physical behaviours that are to be expected.

In Chapter 4 we fitted the seven model parameters to the carbon dioxide data taken from NIST, itself calculated using the Span–Wagner Equation of State [35]. This data came in the form of homogeneous phase volume–pressure isotherms and pure carbon dioxide two–phase boundary volumes and vapour pressures. We deployed the methodologies outlined in Chapter 2 to find values for the seven parameters which would allow the model to most closely match the behaviour given by the NIST data. For fitting the critical temperature isotherm, a strong emphasis was placed on excellent agreement with the pressure (density) data to ensure qualitative behaviour was described accurately, including an excellent estimation of the critical point itself and of the density data either side of the critical volume. The variation of each parameter with temperature was obtained through a sequence of small perturbations in temperature, followed by recalibration of the parameters through local root finding at the new temperature. The disagreement with the pressure and co-existence data was also measured at each subsequent temperature to ensure we had generated a minimum of the error function in which the proposed equation closely resembled the behaviour described by the NIST database. This allowed us to formulate the temperature dependence of each parameter, and in this way the model for describing pure carbon dioxide was finalised. The performance of the model in this case was seen to be well within our aims and we had a paper on this stage of the work published [40] in early 2013.

In Chapter 5 we carried out the fitting to the various mixture data we had col-

lected for the three binary systems we were targeting. We were able to perform the fitting with a high degree of accuracy at a range of temperature points, and as a result draw up a temperature dependence for each model parameter between these temperatures. In doing so, we were able to show that the overall behaviour of the model between and in the vicinity of points at which a fitting had been possible was very good, and we took confidence from this as it showed that our equation was powerful enough to capture the behaviour of these binary mixtures where such data existed.

For the carbon dioxide–nitrogen fitting, we could start to see some of the implications of the current state of the literature data. Indeed, of the five temperature points at which VLE data was available for this mixture, only two of them within the relevant temperature range also had homogeneous mixture density data to allow us to conduct a fitting. This had previously necessitated the development of our methods for coexisting volume estimation and homogeneous density estimation.

In extending the work to the carbon dioxide–hydrogen mixture, we again faced difficulties: There were only two temperature points at which VLE data containing the full array of thermodynamic information was given, one of these being below the range of interest. Furthermore, there were no temperatures at which both homogeneous mixture density and VLE data, whether with volumes or not, existed. Without our volume estimation technique, we would therefore have only been able to fit a single temperature point in a meaningful way. At this temperature, the model was found to give an excellent description of the behaviour, and using the estimation techniques we were able to get acceptable descriptions at some other temperature points.

The carbon dioxide–oxygen binary mixture data was in a similar state. This time there was only a single temperature point at which the full array of VLE information was given, and again, no temperature points at which both VLE and homogeneous density data simultaneously existed. At the few temperature points at which we had been able to perform a fitting, these were again found to be very good.

6.3 Strengths of the Proposed Model

As we can see from Tables 4.2, 4.3, and Figure 4.32, our proposed equation of state appeared to have great potential when compared directly with the PREoS, even though it possessed only slight extra functional complexity. It gave a consistently

superior description of the pressure–density behaviour throughout the CCS–relevant temperature range, which we found to be very close to that of the SWEoS at all but a few points. It also gave, even in the worst cases, a comparably accurate description of the phase behaviour to the PREoS, although usually far superior. For descriptions of the bubble line, which we considered to be the more important consideration for CCS pipeline transport, the predictions were significantly better than the PREoS at all times, again approaching the SWEoS in terms of accuracy in some places.

From our analysis, it seemed the only place the proposed model did not match the high standard exhibited elsewhere was in the immediate vicinity of the critical point. As had been demonstrated in our paper, the model had flexibility to predict the critical point exactly, but this came at the cost of a worse performance around the critical point, so for this thesis we deliberately imposed a high tariff on the model exhibiting a generally more consistent behaviour. The table and figures would seem to suggest that there was nowhere in the window 260–335K, 1–200bar where the PREoS described the pressure behaviour more accurately than the proposed EoS. Moreover, the dominance of the proposed equation suggested that we had established an excellent starting point from which to extend this model to descriptions of physical behaviour of CCS–relevant mixtures.

For creating descriptions of the binary mixtures in those cases where we had been able to perform a fitting to a more comprehensive data set, superior agreements, such as in the case of the oxygen mixture at 273.15K were gained. When possible, we found the average percentage errors to fall within or very close to our target range. This was a sign that we had proposed both a model that had sufficient scope to achieve the aims, and a method by which to develop and calibrate it.

A further strength of the methods we used to develop our model was that they are general enough to allow scope for new data to be incorporated at the fitting stage as and when it becomes available. This generality means that we would expect our method to allow the proposed model to be continually refined and updated as new data is published.

6.4 Limitation of the Proposed Model

We are clear that the proposed model did not generalise to all temperatures within the range of interest for binary mixtures. Nevertheless, we were able to clearly

identify why this was the case, and in Section 6.5 we suggest actions that could be taken to further the work we have done. The development of auxiliary methods such as that for the estimation of volumes at the phase boundary and that relating pure and mixture fugacities would enable this to be done. As such, we are confident that we have put everything in place so that once the correct thermodynamic data becomes available, our methods can be employed exactly as prescribed in this thesis to bring about the equation of state currently needed for understanding CCS pipeline transport.

6.5 Future Work

We are confident that the the work we have carried out in this EngD makes a major contribution towards furthering the understanding of the physical behaviour of CO₂-rich mixtures as relevant to CCS pipeline transport.

We suggest the following tasks which could be carried out, either in progression of this work, or generally for the deepening of understanding in this area. To begin with, the following important thermodynamic measurements could be conducted:

- CO₂-N₂: A range of homogeneous density-pressure measurements in the liquid phase upto a pressure of 80MPa at 303.3K and 301.3K (to complement the VLE data given in [91]), 298.15K (to complement the partial VLE data given in [104]), 293.3K (to complement the partial VLE data given in [106]), 273.15K (to complement the VLE data given in [54]), and at 270K (to complement the partial VLE data given in [98]). These should be carried out at a range of nitrogen compositions up to 50%. Also needed are the volumetric measurements to complement the currently available VLE data in which volumes are not quoted.
- CO₂-H₂: A range of homogeneous density-pressure measurements in the liquid phase upto a pressure of 80MPa at 298.15K (to complement the VLE data given in [90]), 290K, 280K, 270K, and 260K (to complement the partial VLE data given in [110]), at a range of nitrogen compositions, and the missing VLE volumes in these cases.
- CO₂-O₂: Phase boundaries at a range of temperatures between 303.22K and 283.15K to complement the homogeneous density data given in [109] and to bridge the large gap to the data at 283.15K in [112]. Also a range of homogeneous density-pressure measurements in the liquid phase upto a pressure of 80MPa at 283.15K (to complement the partial VLE data given in [112]),

273.15K (to complement the VLE data given in [54]), and 263.15K (to complement the partial VLE data given in [112]).

The above measurements are suggested as this would then give a vast increase in the amount of relevant thermodynamic data which the model parameters could be fit to. In light of the suggested measurements, this would be particularly true throughout the range of temperatures and pressures identified throughout this work as being of particular relevance. The fitted parameter values would then have been allowed to take account for describing both types of behaviour, and owing to the relatively small temperature jumps between each measurement, a suitable temperature dependence could be fit to the parameters in each case. With this having been done, it would then be possible to finalise the original aims set out at the start of this work. We highlight that the methods described in this thesis can be used to generate the full binary model descriptions.

A further potential spin-off from this project as a substitute for the suggestion of certain experimental measurements being taken would be to generate these data by using molecular simulation techniques [113]. The advantage of this would be that such methods are less costly, time-consuming, and resource intensive than acquiring laboratory equipment, setting up, and physically taking measurements, and there is seen to be a good performance of such methods. This could produce the data which would then allow for an improved fitting of our model. As a slight generalisation to this approach, we feel that another substitute to the volume estimation techniques we developed could be introduced by allowing the optimisation algorithms discussed in Chapter 2 to find values for the missing VLE volumes alongside its search for the model parameters. This would require significant computing power however, as we found that the ability of simulated annealing to find relevant optima diminished very quickly as the number of parameters grew towards ten and beyond.

Subsequently, there is then also a clear need for the equation of state to give descriptions for mixtures containing more than two components. Our work has opened the door to the generalisation to ternary mixture descriptions, and can again act as a very solid foundation for this research, in particular, the methods for developing and relating fugacity expressions would be useful in calculating the VLE properties of such systems.

As the model is developed and the number of mixture components it is able to describe grows, there is also the possibility that our model should be expanded to incorporate the other chemical impurities present in the CCS chain, such as SO_x ,

NO_x , Ar, Hg, and others. Discussion with fellow researchers and experts in this field at conferences confirm there would be demand to drive this development.

Another way in which we felt our work could be continued past the conclusion of this EngD is if the beginning-to-end method we have employed using Wolfram Mathematica could be automated into a single executable programme. The ultimate aim of this expansion would be to allow the proposal of a functional form such as Equation (3.9) and some mixing rules such as equation (5.35), with supplementary homogeneous density and VLE data, of the type specified in the list above, to be processed automatically, as opposed to manually, such as in the methods used in this work, into a usable model. This would give the output of a fully-fledged equation of state much more quickly. The method would carry out fitting at all the temperature points simultaneously, as opposed to one-by-one as was done here, and could incorporate assurances that each model parameter varied smoothly with temperature by imposing high penalties in the error function for high parameter curvature with temperature.

We felt that, whereas our methods of volume estimation were suitable to our needs of creating a framework on which to build the model, that this could also be developed in order to improve accuracy. In particular, some investigation into the role and definition of the quantities ξ_{BP} , ξ_{DP} , and χ_{DP} , introduced in Chapter 5 could be carried out, as there may be applications of this method in other areas of chemistry or thermodynamics.

These are all natural steps to take in continuing the work we have conducted for this EngD.

6.6 Applications of this EngD Research Project

As discussed at length in Chapter 1, there is a pressing need for an equation of state which can simultaneously give accurate descriptions of the thermodynamic behaviour of mixtures of carbon dioxide and impurities whilst also exhibiting sufficient user-friendliness to be employed without restriction. Our project has established a new formulation which we have demonstrated has the flexibility and power to give excellent descriptions of a wide range of behaviours, whilst maintaining enough simplicity for the equation itself to be written on a single line. The requirement for this new equation of state stemmed from the lack of certainty in designing and operating carbon dioxide pipelines for Carbon Capture and Storage. It is our con-

tention that the work presented here, both as it stands and in terms of what it can be developed into has a very direct application to this task. The accuracy the model demonstrated in places where fittings had been possible was such that we feel comfortable in claiming that it can be utilised in the calculation of physical quantities with sufficient accuracy. This is especially so in light of the obvious simplicity of the model we proposed.

With this, and the possible future work highlighted in Section 6.5 as being a direct spin-off of this project, the applications could reach further perhaps than CCS pipelines. The model itself could be implemented in any process in which pressurised carbon dioxide is handled, for example in some other branches of manufacturing such as in the storage stage of CCS, or the food and beverage industry [114]. The methods will potentially have an application to the modelling of many fluid substances in many circumstances.

6.6.1 Industrial Relevance

The link between our work and its intended purpose means there is a clear industrial relevance. We feel this is a key output from this EngD project, in which there is a particular requirement for an industrial focus. Whereas there is room for development of the methods we established, the model itself could be implemented in the CCS industry under very certain conditions immediately, and for cases in which the modelling of pure carbon dioxide is required.

The industrial relevance of our work is not limited to the uses of the proposed equation itself however, as the methods presented here will facilitate investigation into other equations of state, particularly if the future work generalising our methods to ternary mixtures, and automation of the whole process, can be achieved. The clarity of the relations between different fugacity constraints in particular mean that whenever VLE is being investigated, parts of our method can be employed to allow for a more convenient appointment of the outputs required by the user.

Finally, the list of thermodynamic measurements we suggested should itself give focus to those who are in a position to carry them out in producing outputs of relevance to the CCS industry.

6.6.2 Academic Relevance

Despite the focus on industrial benefits inherent to the EngD, there are also a number of academic relevancies of our work. First and foremost, the headway made in understanding how equations of state can be developed that has come about from this work is significant. We feel that we have offered real insight into the behaviour of carbon dioxide mixtures and have pushed forward the boundaries of knowledge in this regard. Through our auxiliary methods we have also offered increased understanding in many areas surrounding that of the physical behaviour of substances.

As an EngD project, there have been, as is to be expected, many tough times in the production of the outputs presented in this thesis. Not least the struggles with manually developing a method for fitting model parameters to physical descriptions. In refining our methods to reduce these struggles and improve flexibility further, we feel that several academic projects can be created as a result. Investigation into, and improvements of our volume estimations, for example, could make for a good Undergraduate or Masters’-level research project, whilst the effect of different equation of state formulations or mixing rules could make for a good follow-up EngD or PhD project, and the automation of the whole process developed here a good and worthwhile post-doc project for someone with the correct programming expertise. All of these would have very useful industrial, commercial and academic consequences.

6.7 Final Thoughts

We set out initially to develop a new equation of state. It quickly became clear during the early days of the project that knowledge surrounding this area was low, and that equations of state which were available did not meet the specifications of CCS pipeline transport. Our aims thus expanded to include a formalisation of the method by which an equation of state can be generated from first principles, and following on from this, we made several important breakthroughs which will have a clear use in both their intended and other areas. As a result of the relative simplicity coupled with the demonstrated performance of the proposed model, we felt that the work conducted as part of this EngD represented a clear step forward in modelling the physical properties of fluid mixtures with an equation of state.

As atmospheric levels of carbon dioxide rise along with continuing dependence on fossil fuels to power the industry which has brought about phenomenal improvements in standards of living; including science and technology, agriculture, transport and

many other areas since the industrial revolution, there have been clear mandates set out, ensuring that this rise cannot do increasing long-term damage to the environment we are so dependent upon. Carbon Capture and Storage is a strategy that promises to reduce the emissions of carbon dioxide, thus minimising the environmental impacts of the methods of energy extraction that support our way of life.

Although many obstacles still stand in the way of CCS being implemented on the required scale, the many usable results presented in this thesis and the possible spin-offs should go some way to helping overcome some of these. In “Modelling CO₂ Transport and the Effect of Impurities”, and through proposing “A New Equation of State for CCS Pipeline Transport”, we hope that our contribution to one small part of a very large and complicated problem can be of some use.

Chapter 7

Appendices

7.1 A Summary of Literature Thermodynamic Data Used for Fitting

7.1.1 Carbon Dioxide–Nitrogen VLE Data

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 0.600 | — | — | 220 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 1.509 | — | — | 220 | 0.9868 | 0.0132 | 0.4482 | 0.5518 | Vol. Est. |
| 3.075 | — | — | 220 | 0.9638 | 0.0362 | 0.2577 | 0.7423 | Vol. Est. |
| 4.595 | — | — | 220 | 0.9399 | 0.0601 | 0.2026 | 0.7974 | Vol. Est. |
| 6.313 | — | — | 220 | 0.9117 | 0.0883 | 0.1786 | 0.8214 | Vol. Est. |
| 8.258 | — | — | 220 | 0.8791 | 0.1209 | 0.1719 | 0.8281 | Vol. Est. |
| 11.114 | — | — | 220 | 0.8258 | 0.1742 | 0.1835 | 0.8165 | Vol. Est. |
| 12.432 | — | — | 220 | 0.7984 | 0.2016 | 0.1972 | 0.8028 | Vol. Est. |
| 13.796 | — | — | 220 | 0.7676 | 0.2324 | 0.2131 | 0.7869 | Vol. Est. |
| 15.506 | — | — | 220 | 0.7229 | 0.2771 | 0.2484 | 0.7516 | Vol. Est. |
| 16.706 | — | — | 220 | 0.6845 | 0.3155 | 0.2785 | 0.7215 | Vol. Est. |
| 1.287 | — | — | 240 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 2.100 | — | — | 240 | 0.9871 | 0.0129 | 0.6688 | 0.3312 | Vol. Est. |
| 3.208 | — | — | 240 | 0.9693 | 0.0307 | 0.4849 | 0.5151 | Vol. Est. |
| 4.089 | — | — | 240 | 0.9546 | 0.0454 | 0.4110 | 0.5890 | Vol. Est. |
| 5.674 | — | — | 240 | 0.9266 | 0.0734 | 0.3428 | 0.6572 | Vol. Est. |
| 6.262 | — | — | 240 | 0.9162 | 0.0838 | 0.3290 | 0.6710 | Vol. Est. |
| 7.235 | — | — | 240 | 0.8978 | 0.1022 | 0.3127 | 0.6873 | Vol. Est. |
| 8.590 | — | — | 240 | 0.8703 | 0.1297 | 0.3019 | 0.6981 | Vol. Est. |
| 9.945 | — | — | 240 | 0.8408 | 0.1592 | 0.3008 | 0.6992 | Vol. Est. |
| 10.728 | — | — | 240 | 0.8225 | 0.1775 | 0.3040 | 0.6960 | Vol. Est. |
| 11.466 | — | — | 240 | 0.8042 | 0.1958 | 0.3103 | 0.6897 | Vol. Est. |
| 12.225 | — | — | 240 | 0.7835 | 0.2165 | 0.3194 | 0.6806 | Vol. Est. |
| 12.659 | — | — | 240 | 0.7704 | 0.2296 | 0.3255 | 0.6745 | Vol. Est. |
| 13.865 | — | — | 240 | 0.7304 | 0.2696 | 0.3483 | 0.6517 | Vol. Est. |
| 14.472 | — | — | 240 | 0.7056 | 0.2944 | 0.3712 | 0.6288 | Vol. Est. |
| 15.424 | — | — | 240 | 0.6509 | 0.3491 | 0.4071 | 0.5929 | Vol. Est. |
| 15.768 | — | — | 240 | 0.6184 | 0.3816 | 0.4367 | 0.5633 | Vol. Est. |
| 16.147 | — | — | 240 | 0.5223 | 0.4777 | 0.4798 | 0.5202 | Vol. Est. |

Data summarised from Table II of AlSahhaf83 [115]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 6.205 | — | — | 230 | 0.9188 | 0.0812 | 0.2527 | 0.7473 | Vol. Est. |
| 8.619 | — | — | 230 | 0.8638 | 0.1362 | 0.2340 | 0.7660 | Vol. Est. |
| 9.652 | — | — | 230 | 0.8545 | 0.1455 | 0.2402 | 0.7598 | Vol. Est. |
| 8.963 | — | — | 250 | 0.8606 | 0.1394 | 0.3858 | 0.6142 | Vol. Est. |
| 10.342 | — | — | 250 | 0.8233 | 0.1767 | 0.3838 | 0.6162 | Vol. Est. |

Data summarised from TABLE 1 of AlSahhaf90 [116]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 6.88 | — | — | 301.3 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 7.22 | 67.2 | 139 | 301.3 | 0.9931 | 0.0069 | 0.9848 | 0.0152 | Yes |
| 7.33 | 68.3 | 132 | 301.3 | 0.9899 | 0.0101 | 0.9794 | 0.0206 | Yes |
| 7.61 | 69.6 | 122 | 301.3 | 0.9818 | 0.0182 | 0.9674 | 0.0326 | Yes |
| 7.90 | 74 | 114 | 301.3 | 0.9742 | 0.0258 | 0.9610 | 0.0390 | Yes |
| 8.01 | 81.3 | 106 | 301.3 | 0.9652 | 0.0348 | 0.9611 | 0.0389 | Yes |
| 8.05 | 90.7 | 90.7 | 301.3 | 0.9621 | 0.0379 | 0.9621 | 0.0379 | Yes |
| 7.27 | 86.2 | 138 | 303.3 | 0.9987 | 0.0013 | 0.9977 | 0.0023 | Yes |
| 7.44 | 74 | 128 | 303.3 | 0.9940 | 0.0060 | 0.9904 | 0.0096 | Yes |
| 7.53 | 75.8 | 125 | 303.3 | 0.9914 | 0.0086 | 0.9867 | 0.0133 | Yes |
| 7.54 | 75.7 | 122 | 303.3 | 0.9910 | 0.0090 | 0.9864 | 0.0136 | Yes |
| 7.61 | 77.2 | 118 | 303.3 | 0.9893 | 0.0107 | 0.9847 | 0.0153 | Yes |
| 7.73 | 81.9 | 108 | 303.3 | 0.9853 | 0.0147 | 0.9811 | 0.0189 | Yes |
| 7.79 | 90 | 90 | 303.3 | 0.9816 | 0.0184 | 0.9816 | 0.0184 | Yes |

Data summarised from TABLE 2 of Bian93 [91]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|------------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 2.4216675 | 0.000634 | — | 253.15 | — | — | 0.868 | 0.132 | No |
| 2.5432575 | 0.000647 | — | 253.15 | — | — | 0.826 | 0.174 | No |
| 2.9080275 | 0.00055 | — | 253.15 | — | — | 0.757 | 0.243 | No |
| 3.6375675 | 0.000437 | — | 253.15 | — | — | 0.653 | 0.347 | No |
| 4.7521425 | 0.000336 | — | 253.15 | — | — | 0.566 | 0.434 | No |
| 6.8293050 | 0.000223 | — | 253.15 | — | — | 0.466 | 0.534 | No |
| 8.8456725 | — | — | 253.15 | — | — | 0.432 | 0.568 | No |
| 8.9773950 | 0.0000445 | — | 253.15 | 0.868 | 0.132 | — | — | No |
| 10.6188600 | 0.0000459 | — | 253.15 | 0.826 | 0.174 | — | — | No |
| 11.5510500 | — | — | 253.15 | — | — | 0.432 | 0.568 | No |
| 12.7872150 | 0.0000496 | — | 253.15 | 0.757 | 0.243 | — | — | No |
| 13.1114550 | — | 0.0000934 | 253.15 | — | — | 0.466 | 0.534 | No |
| 14.3172225 | 0.0000572 | — | 253.15 | 0.653 | 0.347 | — | — | No |
| 14.3577525 | — | 0.0000687 | 253.15 | — | — | 0.566 | 0.434 | No |
| 3.4957125 | — | 0.000445 | 273.15 | — | — | 1.000 | 0.000 | No |
| 3.5058450 | 0.0000476 | — | 273.15 | 1.000 | 0.000 | — | — | No |
| 3.9111450 | — | 0.000396 | 273.15 | — | — | 0.929 | 0.071 | No |
| 4.3063125 | — | 0.00036 | 273.15 | — | — | 0.872 | 0.128 | No |
| 5.7349950 | — | 0.000253 | 273.15 | — | — | 0.746 | 0.254 | No |
| 6.6063900 | — | 0.000221 | 273.15 | — | — | 0.694 | 0.306 | No |
| 7.1130150 | 0.0000489 | — | 273.15 | 0.929 | 0.071 | — | — | No |
| 8.7544800 | — | 0.000155 | 273.15 | — | — | 0.633 | 0.367 | No |
| 9.4536225 | 0.0000519 | — | 273.15 | 0.872 | 0.128 | — | — | No |
| 10.8924375 | — | 0.000109 | 273.15 | — | — | 0.633 | 0.367 | No |
| 11.8043625 | 0.0000669 | 0.000081 | 273.15 | 0.746 | 0.254 | 0.694 | 0.306 | No |
| 5.0966475 | — | 0.000272 | 288.15 | — | — | 1.000 | 0.000 | No |
| 5.1169125 | 0.0000531 | — | 288.15 | 1.000 | 0.000 | — | — | No |
| 5.6944650 | — | 0.000239 | 288.15 | — | — | 0.940 | 0.060 | No |
| 6.2517525 | — | 0.000213 | 288.15 | — | — | 0.897 | 0.103 | No |
| 6.7381125 | — | 0.000195 | 288.15 | — | — | 0.868 | 0.132 | No |
| 7.1839425 | — | 0.000178 | 288.15 | — | — | 0.845 | 0.155 | No |
| 7.5892425 | — | 0.000166 | 288.15 | — | — | 0.827 | 0.173 | No |
| 7.7817600 | 0.0000567 | — | 288.15 | 0.940 | 0.060 | — | — | No |
| 8.1060000 | — | 0.00015 | 288.15 | — | — | 0.812 | 0.188 | No |
| 8.3289150 | — | 0.000143 | 288.15 | — | — | 0.806 | 0.194 | No |
| 8.5113000 | — | 0.000137 | 288.15 | — | — | 0.801 | 0.199 | No |
| 9.0685875 | — | 0.000118 | 288.15 | — | — | 0.798 | 0.202 | No |
| 9.0888525 | 0.0000625 | — | 288.15 | 0.897 | 0.103 | — | — | No |
| 9.4637550 | — | 0.000107 | 288.15 | — | — | 0.801 | 0.199 | No |
| 9.5752125 | — | 0.000102 | 288.15 | — | — | 0.806 | 0.194 | No |
| 9.6258750 | 0.00007 | — | 288.15 | 0.868 | 0.132 | — | — | No |
| 9.6664050 | — | 0.0000974 | 288.15 | — | — | 0.812 | 0.188 | No |
| 9.7575975 | 0.0000785 | 0.0000879 | 288.15 | 0.845 | 0.155 | 0.827 | 0.173 | No |

Data summarised from Table 1 of Arai71 [53]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 1.784 | — | — | 250 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 2.599 | — | — | 250 | 0.9864 | 0.0136 | 0.7439 | 0.2561 | Vol. Est. |
| 3.688 | — | — | 250 | 0.9669 | 0.0331 | 0.5761 | 0.4239 | Vol. Est. |
| 4.589 | — | — | 250 | 0.9512 | 0.0488 | 0.4999 | 0.5001 | Vol. Est. |
| 5.541 | — | — | 250 | 0.9336 | 0.0664 | 0.4506 | 0.5494 | Vol. Est. |
| 6.597 | — | — | 250 | 0.9130 | 0.0870 | 0.4151 | 0.5849 | Vol. Est. |
| 7.532 | — | — | 250 | 0.8931 | 0.1069 | 0.3951 | 0.6049 | Vol. Est. |
| 9.632 | — | — | 250 | 0.8468 | 0.1532 | 0.3777 | 0.6223 | Vol. Est. |
| 11.151 | — | — | 250 | 0.8069 | 0.1931 | 0.3837 | 0.6163 | Vol. Est. |
| 11.936 | — | — | 250 | 0.7827 | 0.2173 | 0.3937 | 0.6063 | Vol. Est. |
| 13.416 | — | — | 250 | 0.7292 | 0.2708 | 0.4273 | 0.5727 | Vol. Est. |
| 14.066 | — | — | 250 | 0.6992 | 0.3008 | 0.4563 | 0.5437 | Vol. Est. |
| 3.200 | — | — | 270 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 4.857 | — | — | 270 | 0.9684 | 0.0316 | 0.7577 | 0.2423 | Vol. Est. |
| 6.084 | — | — | 270 | 0.9439 | 0.0561 | 0.6691 | 0.3309 | Vol. Est. |
| 7.650 | — | — | 270 | 0.9099 | 0.0901 | 0.6058 | 0.3942 | Vol. Est. |
| 9.102 | — | — | 270 | 0.8721 | 0.1279 | 0.5795 | 0.4205 | Vol. Est. |

Data summarised from Table 1 of Brown89-I [95]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 0.492 | — | — | 220 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 1.012 | — | — | 220 | — | — | 0.6285 | 0.3715 | No |
| 1.094 | — | — | 220 | — | — | 0.5874 | 0.4126 | No |
| 1.195 | — | — | 220 | — | — | 0.5452 | 0.4548 | No |
| 1.373 | — | — | 220 | 0.9892 | 0.0108 | 0.4826 | 0.5174 | Vol. Est. |
| 1.675 | — | — | 220 | — | — | 0.4080 | 0.5920 | No |
| 1.751 | — | — | 220 | — | — | 0.3946 | 0.6054 | No |
| 1.795 | — | — | 220 | — | — | 0.3864 | 0.6136 | No |
| 2.016 | — | — | 220 | — | — | 0.3521 | 0.6479 | No |
| 2.363 | — | — | 220 | — | — | 0.3124 | 0.6876 | No |
| 2.457 | — | — | 220 | 0.9731 | 0.0269 | 0.3029 | 0.6971 | Vol. Est. |
| 3.444 | — | — | 220 | — | — | 0.2402 | 0.7598 | No |
| 3.465 | — | — | 220 | — | — | 0.2390 | 0.7610 | No |
| 3.775 | — | — | 220 | — | — | 0.2263 | 0.7737 | No |
| 4.029 | — | — | 220 | — | — | 0.2179 | 0.7821 | No |
| 5.207 | — | — | 220 | — | — | 0.1919 | 0.8081 | No |
| 5.270 | — | — | 220 | — | — | 0.1906 | 0.8094 | No |
| 5.313 | — | — | 220 | — | — | 0.1904 | 0.8096 | No |
| 5.466 | — | — | 220 | — | — | 0.1886 | 0.8114 | No |
| 5.985 | — | — | 220 | — | — | 0.1818 | 0.8182 | No |
| 5.993 | — | — | 220 | 0.9170 | 0.0830 | 0.1850 | 0.8150 | Vol. Est. |
| 6.746 | — | — | 220 | — | — | 0.1768 | 0.8232 | No |
| 7.111 | — | — | 220 | — | — | 0.1747 | 0.8253 | No |
| 7.143 | — | — | 220 | — | — | 0.1750 | 0.8250 | No |
| 7.151 | — | — | 220 | — | — | 0.1744 | 0.8256 | No |
| 7.281 | — | — | 220 | — | — | 0.1745 | 0.8255 | No |
| 7.310 | — | — | 220 | — | — | 0.1742 | 0.8258 | No |
| 7.485 | — | — | 220 | 0.8908 | 0.1092 | 0.1738 | 0.8262 | Vol. Est. |
| 7.910 | — | — | 220 | — | — | 0.1732 | 0.8268 | No |
| 8.625 | — | — | 220 | — | — | 0.1734 | 0.8266 | No |
| 9.098 | — | — | 220 | 0.8662 | 0.1338 | 0.1736 | 0.8264 | Vol. Est. |
| 9.198 | — | — | 220 | — | — | 0.1742 | 0.8258 | No |
| 10.320 | — | — | 220 | — | — | 0.1792 | 0.8208 | No |
| 10.460 | — | — | 220 | — | — | 0.1801 | 0.8199 | No |
| 10.894 | — | — | 220 | — | — | 0.1830 | 0.8170 | No |
| 11.311 | — | — | 220 | — | — | 0.1864 | 0.8136 | No |
| 11.478 | — | — | 220 | — | — | 0.1882 | 0.8118 | No |
| 11.968 | — | — | 220 | — | — | 0.1924 | 0.8076 | No |
| 11.995 | — | — | 220 | 0.8097 | 0.1903 | 0.1920 | 0.8080 | Vol. Est. |
| 12.677 | — | — | 220 | — | — | 0.2009 | 0.7991 | No |
| 12.962 | — | — | 220 | — | — | 0.2036 | 0.7964 | Vol. Est. |
| 3.202 | — | — | 270 | 1.0000 | 0.0000 | 0.0000 | 0.0000 | Vol. Est. |
| 4.334 | — | — | 270 | — | — | 0.8170 | 0.1830 | No |
| 4.686 | — | — | 270 | — | — | 0.7788 | 0.2212 | No |
| 5.074 | — | — | 270 | — | — | 0.7435 | 0.2565 | No |
| 5.779 | — | — | 270 | 0.9502 | 0.0498 | 0.6913 | 0.3087 | Vol. Est. |
| 5.860 | — | — | 270 | — | — | 0.6861 | 0.3139 | No |
| 6.182 | — | — | 270 | 0.9434 | 0.0566 | 0.6678 | 0.3322 | Vol. Est. |
| 6.436 | — | — | 270 | — | — | 0.6544 | 0.3456 | No |
| 7.165 | — | — | 270 | 0.9230 | 0.0770 | 0.6253 | 0.3747 | Vol. Est. |
| 7.289 | — | — | 270 | — | — | 0.6215 | 0.3785 | No |
| 7.546 | — | — | 270 | 0.9139 | 0.0861 | 0.6121 | 0.3879 | Vol. Est. |
| 7.766 | — | — | 270 | — | — | 0.6070 | 0.3930 | No |
| 8.289 | — | — | 270 | 0.8945 | 0.1055 | 0.5951 | 0.4049 | Vol. Est. |
| 8.476 | — | — | 270 | 0.8910 | 0.1090 | 0.5905 | 0.4095 | Vol. Est. |
| 9.001 | — | — | 270 | 0.8770 | 0.1230 | 0.5852 | 0.4148 | Vol. Est. |
| 9.283 | — | — | 270 | — | — | 0.5824 | 0.4176 | No |
| 9.586 | — | — | 270 | 0.8612 | 0.1388 | 0.5814 | 0.4186 | Vol. Est. |
| 9.618 | — | — | 270 | — | — | 0.5796 | 0.4204 | No |
| 10.193 | — | — | 270 | 0.8428 | 0.1572 | 0.5808 | 0.4192 | Vol. Est. |
| 10.393 | — | — | 270 | — | — | 0.5826 | 0.4174 | No |

Data summarised from TABLE 1 of Brown89-II [96]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 3.48530 | 0.00004735 | 0.0004505 | 273.15 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Yes |
| 3.79212 | 0.00004760 | 0.0004240 | 274.15 | 0.9942 | 0.0058 | 0.9470 | 0.0530 | Yes |
| 4.13685 | 0.00004788 | 0.0003970 | 275.15 | 0.9878 | 0.0122 | 0.8970 | 0.1030 | Yes |
| 4.48159 | 0.00004816 | 0.0003700 | 276.15 | 0.9810 | 0.0190 | 0.8550 | 0.1450 | Yes |
| 4.82633 | 0.00004845 | 0.0003430 | 277.15 | 0.9745 | 0.0255 | 0.8190 | 0.1810 | Yes |
| 5.17107 | 0.00004875 | 0.0003160 | 278.15 | 0.9680 | 0.0320 | 0.7905 | 0.2095 | Yes |
| 5.51581 | 0.00004805 | 0.0002920 | 279.15 | 0.9610 | 0.0390 | 0.7640 | 0.2360 | Yes |
| 5.86054 | 0.00004940 | 0.0002690 | 280.15 | 0.9540 | 0.0460 | 0.7393 | 0.2607 | Yes |
| 6.20528 | 0.00004970 | 0.0002520 | 281.15 | 0.9465 | 0.0535 | 0.7164 | 0.2836 | Yes |
| 6.55002 | 0.00005005 | 0.0002380 | 282.15 | 0.9393 | 0.0607 | 0.6962 | 0.3038 | Yes |
| 6.89476 | 0.00005040 | 0.0002260 | 283.15 | 0.9315 | 0.0685 | 0.6782 | 0.3218 | Yes |
| 7.23950 | 0.00005080 | 0.0002130 | 284.15 | 0.9236 | 0.0764 | 0.6634 | 0.3366 | Yes |
| 7.58423 | 0.00005118 | 0.0002020 | 285.15 | 0.9142 | 0.0858 | 0.6516 | 0.3484 | Yes |
| 7.92897 | 0.00005158 | 0.0001910 | 286.15 | 0.9057 | 0.0943 | 0.6412 | 0.3588 | Yes |
| 8.27371 | 0.00005200 | 0.0001810 | 287.15 | 0.8970 | 0.1030 | 0.6325 | 0.3675 | Yes |
| 8.61845 | 0.00005240 | 0.0001710 | 288.15 | 0.8885 | 0.1115 | 0.6261 | 0.3739 | Yes |
| 8.96318 | 0.00005288 | 0.0001620 | 289.15 | 0.8798 | 0.1202 | 0.6210 | 0.3790 | Yes |
| 9.30792 | 0.00005338 | 0.0001550 | 290.15 | 0.8703 | 0.1297 | 0.6175 | 0.3825 | Yes |
| 9.65266 | 0.00005395 | 0.0001470 | 291.15 | 0.8610 | 0.1390 | 0.6148 | 0.3852 | Yes |
| 9.99740 | 0.00005460 | 0.0001390 | 292.15 | 0.8508 | 0.1492 | 0.6140 | 0.3860 | Yes |
| 10.34214 | 0.00005545 | 0.0001310 | 293.15 | 0.8393 | 0.1607 | 0.6158 | 0.3842 | Yes |
| 10.68687 | 0.00005660 | 0.0001230 | 294.15 | 0.8253 | 0.1747 | 0.6200 | 0.3800 | Yes |
| 11.03161 | 0.00005820 | 0.0001150 | 295.15 | 0.8098 | 0.1902 | 0.6274 | 0.3726 | Yes |
| 11.37635 | 0.00006045 | 0.0001060 | 296.15 | 0.7905 | 0.2095 | 0.6384 | 0.3616 | Yes |
| 11.72109 | 0.00006375 | 0.0000960 | 297.15 | 0.7640 | 0.2360 | 0.6572 | 0.3428 | Yes |
| 11.89346 | 0.00006760 | 0.0000882 | 298.15 | 0.7432 | 0.2568 | 0.6776 | 0.3224 | Yes |
| 11.99688 | 0.00007750 | 0.0000775 | 299.15 | 0.7074 | 0.2926 | 0.7074 | 0.2926 | Yes |

Data summarised from Table III of Muirbrook64 [54]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|------------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 3.1988306 | — | — | 270 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 3.4247853 | — | — | 270 | 0.9960 | 0.0040 | 0.9528 | 0.0472 | Vol. Est. |
| 3.6274354 | — | — | 270 | 0.9922 | 0.0078 | 0.9150 | 0.0850 | Vol. Est. |
| 3.7996879 | — | — | 270 | 0.9892 | 0.0108 | 0.8860 | 0.1140 | Vol. Est. |
| 3.9516754 | — | — | 270 | 0.9900 | 0.0100 | 0.8669 | 0.1331 | Vol. Est. |
| 4.1219014 | — | — | 270 | 0.9832 | 0.0168 | 0.8402 | 0.1598 | Vol. Est. |
| 4.2049879 | — | — | 270 | 0.9818 | 0.0182 | 0.8317 | 0.1683 | Vol. Est. |
| 4.2809817 | — | — | 270 | 0.9803 | 0.0197 | 0.8217 | 0.1783 | Vol. Est. |
| 4.5596255 | — | — | 270 | 0.9750 | 0.0250 | 0.7885 | 0.2115 | Vol. Est. |
| 4.5900230 | — | — | 270 | 0.9737 | 0.0263 | 0.7844 | 0.2156 | Vol. Est. |
| 4.7602490 | — | — | 270 | 0.9711 | 0.0289 | 0.7677 | 0.2323 | Vol. Est. |
| 4.7744345 | — | — | 270 | 0.9708 | 0.0292 | 0.7675 | 0.2325 | Vol. Est. |
| 5.1523768 | — | — | 270 | 0.9632 | 0.0368 | 0.7326 | 0.2674 | Vol. Est. |
| 5.6985186 | — | — | 270 | 0.9524 | 0.0476 | 0.6931 | 0.3069 | Vol. Est. |
| 6.0491031 | — | — | 270 | 0.9455 | 0.0545 | 0.6720 | 0.3280 | Vol. Est. |
| 6.0795006 | — | — | 270 | 0.9440 | 0.0560 | 0.6710 | 0.3290 | Vol. Est. |
| 6.4442706 | — | — | 270 | 0.9370 | 0.0630 | 0.6530 | 0.3470 | Vol. Est. |
| 7.0927507 | — | — | 270 | 0.9222 | 0.0778 | 0.6230 | 0.3770 | Vol. Est. |
| 7.7209658 | — | — | 270 | 0.9079 | 0.0921 | 0.6039 | 0.3961 | Vol. Est. |
| 8.3795783 | — | — | 270 | 0.8920 | 0.1080 | 0.5874 | 0.4126 | Vol. Est. |
| 8.6126259 | — | — | 270 | 0.8858 | 0.1142 | 0.5861 | 0.4139 | Vol. Est. |
| 8.9824621 | — | — | 270 | 0.8769 | 0.1231 | 0.5810 | 0.4190 | Vol. Est. |
| 9.2915034 | — | — | 270 | 0.8681 | 0.1319 | 0.5827 | 0.4173 | Vol. Est. |
| 9.6258760 | — | — | 270 | 0.8570 | 0.1430 | 0.5790 | 0.4210 | Vol. Est. |
| 10.2044418 | — | — | 270 | 0.8415 | 0.1585 | 0.5812 | 0.4188 | Vol. Est. |
| 10.7141066 | — | — | 270 | 0.8231 | 0.1769 | 0.5866 | 0.4134 | Vol. Est. |
| 11.0525321 | — | — | 270 | 0.8096 | 0.1904 | 0.5906 | 0.4094 | Vol. Est. |
| 11.1457511 | — | — | 270 | 0.8050 | 0.1950 | 0.5920 | 0.4080 | Vol. Est. |
| 11.2521424 | — | — | 270 | 0.8014 | 0.1986 | 0.5939 | 0.4061 | Vol. Est. |
| 11.5490246 | — | — | 270 | 0.7858 | 0.2142 | 0.6014 | 0.3986 | Vol. Est. |
| 11.8175359 | — | — | 270 | — | — | 0.6143 | 0.3857 | No |
| 11.8864369 | — | — | 270 | 0.7668 | 0.2332 | 0.6200 | 0.3800 | Vol. Est. |
| 11.8864369 | — | — | 270 | 0.7640 | 0.2360 | 0.6192 | 0.3808 | Vol. Est. |
| 11.9482452 | — | — | 270 | 0.7514 | 0.2486 | 0.6238 | 0.3762 | Vol. Est. |
| 12.0242389 | — | — | 270 | 0.7546 | 0.2454 | 0.6280 | 0.3720 | Vol. Est. |
| 12.0728749 | — | — | 270 | 0.7495 | 0.2505 | 0.6336 | 0.3664 | Vol. Est. |
| 12.1346832 | — | — | 270 | 0.7444 | 0.2556 | 0.6360 | 0.3640 | Vol. Est. |
| 12.1964915 | — | — | 270 | — | — | 0.6476 | 0.3524 | No |
| 12.3413862 | — | — | 270 | 0.6470 | 0.3530 | 0.6470 | 0.3530 | Vol. Est. |

Data summarised from Table III, IV, V, and VIII of Somait78 [97]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 5.0 | — | — | 223.25 | 0.9327 | 0.0673 | 0.2171 | 0.7829 | Vol. Est. |
| 10.0 | — | — | 223.25 | 0.8444 | 0.1556 | 0.1994 | 0.8006 | Vol. Est. |
| 5.0 | — | — | 248.15 | 0.9425 | 0.0575 | 0.4562 | 0.5438 | Vol. Est. |
| 10.0 | — | — | 248.15 | 0.8384 | 0.1616 | 0.3656 | 0.6344 | Vol. Est. |
| 5.0 | — | — | 273.15 | 0.9709 | 0.0291 | 0.7919 | 0.2081 | Vol. Est. |
| 7.5 | — | — | 273.15 | 0.9168 | 0.0832 | 0.6618 | 0.3382 | Vol. Est. |

Data summarised from TABLE 5 of Weber84 [102]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 21.254 | 5.03423E-05 | — | 210.095 | 0.3991 | 0.6009 | — | — | No |
| 19.833 | 5.34874E-05 | — | 216.264 | 0.3991 | 0.6009 | — | — | No |
| 17.891 | 6.04522E-05 | — | 226.753 | 0.3991 | 0.6009 | — | — | No |
| 17.130 | 6.42963E-05 | — | 230.785 | 0.3991 | 0.6009 | — | — | No |
| 16.485 | 6.83995E-05 | — | 235.038 | 0.3991 | 0.6009 | — | — | No |
| 15.899 | 7.2759E-05 | — | 238.532 | 0.3991 | 0.6009 | — | — | No |
| 20.624 | 4.98853E-05 | — | 214.188 | 0.4459 | 0.5541 | — | — | No |
| 18.891 | 5.40103E-05 | — | 221.551 | 0.4459 | 0.5541 | — | — | No |
| 18.101 | 5.61892E-05 | — | 225.488 | 0.4459 | 0.5541 | — | — | No |
| 21.416 | 4.53679E-05 | — | 208.929 | 0.5037 | 0.4963 | — | — | No |
| 19.417 | 4.84426E-05 | — | 215.579 | 0.5037 | 0.4963 | — | — | No |
| 18.153 | 5.16556E-05 | — | 224.234 | 0.5037 | 0.4963 | — | — | No |
| 17.220 | 5.50297E-05 | — | 231.416 | 0.5037 | 0.4963 | — | — | No |
| 15.842 | 6.25939E-05 | — | 242.167 | 0.5037 | 0.4963 | — | — | No |
| 15.282 | 6.67958E-05 | — | 246.524 | 0.5037 | 0.4963 | — | — | No |
| 14.578 | 7.12758E-05 | — | 250.677 | 0.5037 | 0.4963 | — | — | No |
| 14.376 | 7.58783E-05 | — | 253.563 | 0.5037 | 0.4963 | — | — | No |
| 13.916 | 8.07428E-05 | — | 256.581 | 0.5037 | 0.4963 | — | — | No |
| 13.492 | 8.60511E-05 | — | 259.245 | 0.5037 | 0.4963 | — | — | No |
| 13.121 | 9.16926E-05 | — | 261.559 | 0.5037 | 0.4963 | — | — | No |
| 12.387 | 0.000102638 | — | 264.922 | 0.5037 | 0.4963 | — | — | No |
| 11.614 | 0.000114613 | — | 266.953 | 0.5037 | 0.4963 | — | — | No |
| 10.798 | 0.000128634 | — | 268.039 | 0.5037 | 0.4963 | — | — | No |

Data summarised from Table 5 of Duarte–Garza95–I [77]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 1.0009 | — | — | 220 | 0.9941 | 0.0059 | 0.6326 | 0.3674 | Vol. Est. |
| 1.5094 | — | — | 220 | 0.9866 | 0.0134 | 0.4417 | 0.5583 | Vol. Est. |
| 3.0839 | — | — | 220 | 0.9629 | 0.0371 | 0.2549 | 0.7451 | Vol. Est. |
| 4.5949 | — | — | 220 | 0.9381 | 0.0619 | 0.2014 | 0.7986 | Vol. Est. |
| 6.3075 | — | — | 220 | 0.9084 | 0.0916 | 0.1767 | 0.8233 | Vol. Est. |
| 6.3159 | — | — | 220 | 0.9094 | 0.0906 | 0.1760 | 0.8240 | Vol. Est. |
| 7.9935 | — | — | 220 | 0.8803 | 0.1197 | 0.1685 | 0.8315 | Vol. Est. |
| 8.2669 | — | — | 220 | 0.8802 | 0.1198 | 0.1688 | 0.8312 | Vol. Est. |
| 9.9974 | — | — | 220 | 0.8771 | 0.1229 | 0.1736 | 0.8264 | Vol. Est. |
| 10.0169 | — | — | 220 | 0.8484 | 0.1516 | 0.1742 | 0.8258 | Vol. Est. |
| 10.0257 | — | — | 220 | 0.8476 | 0.1524 | 0.1734 | 0.8266 | Vol. Est. |
| 11.9998 | — | — | 220 | 0.8092 | 0.1908 | 0.1885 | 0.8115 | Vol. Est. |
| 12.4303 | — | — | 220 | 0.8002 | 0.1998 | 0.1930 | 0.8070 | Vol. Est. |
| 13.7768 | — | — | 220 | 0.7690 | 0.2310 | 0.2108 | 0.7892 | Vol. Est. |
| 13.9681 | — | — | 220 | 0.7636 | 0.2364 | 0.2408 | 0.7592 | Vol. Est. |

Data summarised from Tabelle 5.4 of Trappehl87 [117]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 5.11 | — | — | 288.3 | 1.000 | 0.000 | 1.000 | 0.000 | Vol. Est. |
| 6.61 | — | — | 288.3 | 0.965 | 0.035 | 0.875 | 0.125 | Vol. Est. |
| 6.70 | — | — | 288.3 | 0.964 | 0.036 | 0.873 | 0.127 | Vol. Est. |
| 7.61 | — | — | 288.3 | 0.938 | 0.062 | 0.828 | 0.172 | Vol. Est. |
| 7.63 | — | — | 288.3 | 0.936 | 0.064 | 0.820 | 0.180 | Vol. Est. |
| 8.38 | — | — | 288.3 | 0.912 | 0.088 | 0.798 | 0.202 | Vol. Est. |
| 9.01 | — | — | 288.3 | 0.893 | 0.107 | 0.796 | 0.204 | Vol. Est. |
| 9.59 | — | — | 288.3 | 0.860 | 0.140 | 0.807 | 0.193 | Vol. Est. |
| 9.70 | — | — | 288.3 | 0.852 | 0.148 | 0.808 | 0.192 | Vol. Est. |
| 5.72 | — | — | 293.3 | 1.000 | 0.000 | 1.000 | 0.000 | Vol. Est. |
| 6.00 | — | — | 293.3 | 0.995 | 0.005 | 0.977 | 0.023 | Vol. Est. |
| 6.47 | — | — | 293.3 | 0.983 | 0.017 | 0.943 | 0.057 | Vol. Est. |
| 6.49 | — | — | 293.3 | 0.983 | 0.017 | 0.941 | 0.059 | Vol. Est. |
| 6.98 | — | — | 293.3 | 0.971 | 0.029 | 0.912 | 0.088 | Vol. Est. |
| 7.42 | — | — | 293.3 | 0.959 | 0.041 | 0.889 | 0.111 | Vol. Est. |
| 8.10 | — | — | 293.3 | 0.939 | 0.061 | 0.864 | 0.136 | Vol. Est. |
| 8.70 | — | — | 293.3 | 0.924 | 0.076 | 0.863 | 0.137 | Vol. Est. |
| 8.90 | — | — | 293.3 | 0.914 | 0.086 | 0.867 | 0.133 | Vol. Est. |
| 9.03 | — | — | 293.3 | 0.904 | 0.096 | 0.871 | 0.129 | Vol. Est. |
| 9.11 | — | — | 293.3 | 0.884 | 0.116 | 0.884 | 0.116 | Vol. Est. |

Data summarised from TABLE 2 of Xu92 [106]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|---|---|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 3.485580 | — | — | 273.15 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 4.053000 | — | — | 273.15 | 0.9850 | 0.0150 | 0.9036 | 0.0964 | Vol. Est. |
| 4.053000 | — | — | 273.15 | 0.9890 | 0.0110 | 0.9090 | 0.0910 | Vol. Est. |
| 5.066250 | — | — | 273.15 | 0.9690 | 0.0310 | 0.7850 | 0.2150 | Vol. Est. |
| 6.079500 | — | — | 273.15 | 0.9439 | 0.0561 | 0.7100 | 0.2900 | Vol. Est. |
| 6.079500 | — | — | 273.15 | 0.9490 | 0.0510 | 0.7000 | 0.3000 | Vol. Est. |
| 7.092750 | — | — | 273.15 | 0.9290 | 0.0710 | 0.6530 | 0.3470 | Vol. Est. |
| 8.106000 | — | — | 273.15 | 0.9033 | 0.0967 | 0.6300 | 0.3700 | Vol. Est. |
| 8.106000 | — | — | 273.15 | 0.8990 | 0.1010 | 0.6250 | 0.3750 | Vol. Est. |
| 9.119250 | — | — | 273.15 | 0.8740 | 0.1260 | 0.6080 | 0.3920 | Vol. Est. |
| 9.625875 | — | — | 273.15 | 0.8550 | 0.1450 | 0.6100 | 0.3900 | Vol. Est. |
| 10.132500 | — | — | 273.15 | 0.8420 | 0.1580 | 0.6030 | 0.3970 | Vol. Est. |
| 11.145750 | — | — | 273.15 | 0.8000 | 0.2000 | 0.6100 | 0.3900 | Vol. Est. |
| 11.652375 | — | — | 273.15 | 0.7490 | 0.2510 | 0.6440 | 0.3560 | Vol. Est. |
| 11.753700 | — | — | 273.15 | 0.7280 | 0.2720 | 0.6620 | 0.3380 | Vol. Est. |
| 11.824628 | — | — | 273.15 | 0.7030 | 0.2970 | 0.7030 | 0.2970 | Vol. Est. |

Data summarised from Table 1 of Yorizane70 [84]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|---|---|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 4.50 | — | — | 273.2 | 0.980 | 0.020 | 0.846 | 0.154 | Vol. Est. |
| 4.51 | — | — | 273.2 | 0.981 | 0.019 | 0.842 | 0.158 | Vol. Est. |
| 5.09 | — | — | 273.2 | 0.963 | 0.037 | 0.786 | 0.214 | Vol. Est. |
| 5.71 | — | — | 273.2 | 0.946 | 0.054 | 0.736 | 0.264 | Vol. Est. |
| 6.61 | — | — | 273.2 | 0.934 | 0.066 | 0.702 | 0.298 | Vol. Est. |
| 6.70 | — | — | 273.2 | 0.928 | 0.072 | 0.682 | 0.318 | Vol. Est. |
| 7.83 | — | — | 273.2 | 0.895 | 0.105 | 0.644 | 0.356 | Vol. Est. |
| 8.39 | — | — | 273.2 | 0.890 | 0.110 | 0.625 | 0.375 | Vol. Est. |
| 9.95 | — | — | 273.2 | 0.844 | 0.156 | 0.603 | 0.397 | Vol. Est. |
| 9.99 | — | — | 273.2 | 0.853 | 0.147 | 0.614 | 0.386 | Vol. Est. |
| 10.92 | — | — | 273.2 | 0.816 | 0.184 | 0.622 | 0.378 | Vol. Est. |
| 11.45 | — | — | 273.2 | 0.786 | 0.214 | 0.632 | 0.368 | Vol. Est. |
| 6.59 | — | — | 293.2 | 0.979 | 0.021 | 0.933 | 0.067 | Vol. Est. |
| 6.60 | — | — | 293.2 | 0.979 | 0.021 | 0.934 | 0.066 | Vol. Est. |
| 7.56 | — | — | 293.2 | 0.950 | 0.050 | 0.883 | 0.117 | Vol. Est. |
| 7.59 | — | — | 293.2 | 0.951 | 0.049 | 0.882 | 0.118 | Vol. Est. |
| 8.31 | — | — | 293.2 | 0.932 | 0.068 | 0.862 | 0.138 | Vol. Est. |
| 8.33 | — | — | 293.2 | 0.930 | 0.070 | 0.861 | 0.139 | Vol. Est. |
| 8.35 | — | — | 293.2 | 0.930 | 0.070 | 0.860 | 0.140 | Vol. Est. |
| 8.37 | — | — | 293.2 | 0.930 | 0.070 | 0.860 | 0.140 | Vol. Est. |
| 8.43 | — | — | 293.2 | 0.927 | 0.073 | 0.861 | 0.139 | Vol. Est. |
| 8.53 | — | — | 293.2 | 0.923 | 0.077 | 0.857 | 0.143 | Vol. Est. |
| 8.86 | — | — | 293.2 | 0.907 | 0.093 | 0.858 | 0.142 | Vol. Est. |
| 8.91 | — | — | 293.2 | 0.907 | 0.093 | 0.855 | 0.145 | Vol. Est. |
| 9.26 | — | — | 293.2 | 0.898 | 0.102 | 0.855 | 0.145 | Vol. Est. |
| 9.32 | — | — | 293.2 | 0.889 | 0.111 | 0.853 | 0.147 | Vol. Est. |
| 9.37 | — | — | 293.2 | 0.886 | 0.114 | 0.851 | 0.149 | Vol. Est. |
| 9.55 | — | — | 293.2 | 0.882 | 0.118 | 0.850 | 0.150 | Vol. Est. |
| 9.60 | — | — | 293.2 | 0.877 | 0.123 | 0.852 | 0.148 | Vol. Est. |
| 7.40 | — | — | 298.2 | 0.974 | 0.026 | 0.942 | 0.058 | Vol. Est. |
| 7.41 | — | — | 298.2 | 0.973 | 0.027 | 0.943 | 0.057 | Vol. Est. |
| 8.14 | — | — | 298.2 | 0.947 | 0.053 | 0.916 | 0.084 | Vol. Est. |
| 8.17 | — | — | 298.2 | 0.950 | 0.050 | 0.912 | 0.088 | Vol. Est. |
| 8.51 | — | — | 298.2 | 0.933 | 0.067 | 0.902 | 0.098 | Vol. Est. |

Data summarised from Table II of Yorizane85 [104]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-----------|--|--|---------------|-------------------|------------------|-------------------|------------------|--------------------|
| 1.285 | — | — | 240 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 1.696 | — | — | 240 | 0.9906 | 0.0094 | — | — | No |
| 1.707 | — | — | 240 | 0.9918 | 0.0082 | — | — | No |
| 2 | — | — | 240 | 0.9870 | 0.0130 | 0.6814 | 0.3186 | Vol. Est. |
| 2.647 | — | — | 240 | 0.9735 | 0.0265 | — | — | No |
| 3.066 | — | — | 240 | 0.9693 | 0.0307 | — | — | No |
| 3.341 | — | — | 240 | 0.9675 | 0.0325 | — | — | No |
| 8.07 | — | — | 240 | — | — | 0.2998 | 0.7002 | Vol. Est. |
| 10.24 | — | — | 240 | 0.8295 | 0.1705 | — | — | No |
| 10.93 | — | — | 240 | 0.8170 | 0.1830 | 0.3023 | 0.6977 | Vol. Est. |
| 13 | — | — | 240 | 0.7533 | 0.2467 | 0.3308 | 0.6692 | Vol. Est. |
| 3.209 | — | — | 270 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Vol. Est. |
| 3.567 | — | — | 270 | 0.9936 | 0.0064 | 0.9241 | 0.0759 | Vol. Est. |
| 3.688 | — | — | 270 | 0.9904 | 0.0096 | — | — | No |
| 3.719 | — | — | 270 | 0.9912 | 0.0088 | 0.8964 | 0.1036 | Vol. Est. |
| 3.871 | — | — | 270 | 0.9875 | 0.0125 | — | — | No |
| 4.108 | — | — | 270 | 0.9836 | 0.0164 | — | — | No |
| 5.076 | — | — | 270 | 0.9642 | 0.0358 | 0.7371 | 0.2629 | Vol. Est. |
| 6 | — | — | 270 | 0.9470 | 0.0530 | 0.6750 | 0.3250 | Vol. Est. |
| 6.986 | — | — | 270 | — | — | 0.6272 | 0.3728 | Vol. Est. |
| 10.9 | — | — | 270 | 0.8150 | 0.1850 | — | — | No |
| 11.97 | — | — | 270 | 0.7544 | 0.2456 | 0.6178 | 0.3822 | Vol. Est. |

Data summarised from Table 3 and 6 of Yucelen99 [98]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | y_{CO_2} | y_{N_2} | Usable Data Point? |
|-------------|--|--|---------------|-------------------|------------------|-------------------|------------------|--------------------|
| 6.038970596 | — | — | 273.15 | 0.9479 | 0.0521 | 0.7115 | 0.2885 | Vol. Est. |
| 6.028838095 | — | — | 273.15 | 0.9488 | 0.0512 | 0.7080 | 0.2920 | Vol. Est. |
| 4.833202977 | — | — | 273.15 | 0.9735 | 0.0265 | 0.8020 | 0.1980 | Vol. Est. |
| 6.312548123 | — | — | 273.15 | 0.9420 | 0.0580 | 0.6900 | 0.3100 | Vol. Est. |
| 7.994543289 | — | — | 273.15 | 0.9048 | 0.0952 | 0.6270 | 0.3730 | Vol. Est. |
| 9.585345946 | — | — | 273.15 | 0.8592 | 0.1408 | 0.6040 | 0.3960 | Vol. Est. |
| 10.97349858 | — | — | 273.15 | 0.8077 | 0.1923 | 0.6155 | 0.3845 | Vol. Est. |
| 11.66250865 | — | — | 273.15 | 0.7720 | 0.2280 | 0.6460 | 0.3540 | Vol. Est. |
| 11.85502617 | — | — | 273.15 | 0.7025 | 0.2975 | 0.6955 | 0.3045 | Vol. Est. |
| 3.54637535 | — | — | 232.85 | 0.9625 | 0.0375 | 0.3720 | 0.6280 | Vol. Est. |
| 1.763055174 | — | — | 232.85 | 0.9792 | 0.0208 | 0.6280 | 0.3720 | Vol. Est. |
| 11.96648368 | — | — | 232.85 | 0.8320 | 0.1680 | 0.2600 | 0.7400 | Vol. Est. |
| 9.879188475 | — | — | 232.85 | 0.8590 | 0.1410 | — | — | No |
| 7.518315742 | — | — | 232.85 | 0.8910 | 0.1090 | 0.2600 | 0.7400 | Vol. Est. |
| 10.23382601 | — | — | 232.85 | 0.8435 | 0.1565 | 0.2540 | 0.7460 | Vol. Est. |
| 11.1052211 | — | — | 232.85 | 0.8143 | 0.1857 | 0.2470 | 0.7530 | Vol. Est. |
| 12.63522875 | — | — | 232.85 | 0.7810 | 0.2190 | 0.2350 | 0.7650 | Vol. Est. |
| 9.676538455 | — | — | 232.85 | 0.8450 | 0.1550 | 0.2440 | 0.7560 | Vol. Est. |
| 7.974278287 | — | — | 232.85 | 0.8790 | 0.1210 | 0.2440 | 0.7560 | Vol. Est. |
| 6.657053157 | — | — | 232.85 | 0.9040 | 0.0960 | 0.2620 | 0.7380 | Vol. Est. |
| 13.89165887 | — | — | 232.85 | 0.7320 | 0.2680 | 0.2920 | 0.7080 | Vol. Est. |
| 13.06079379 | — | — | 232.85 | 0.7630 | 0.2370 | 0.2530 | 0.7470 | Vol. Est. |
| 1.276695126 | — | — | 218.15 | 0.9910 | 0.0090 | 0.4750 | 0.5250 | Vol. Est. |
| 2.279812725 | — | — | 218.15 | 0.9770 | 0.0230 | 0.2900 | 0.7100 | Vol. Est. |
| 3.85035038 | — | — | 218.15 | 0.9520 | 0.0480 | 0.1960 | 0.8040 | Vol. Est. |
| 5.846453077 | — | — | 218.15 | 0.9340 | 0.0660 | 0.1640 | 0.8360 | Vol. Est. |
| 7.832423273 | — | — | 218.15 | 0.8830 | 0.1170 | 0.1560 | 0.8440 | Vol. Est. |
| 9.869055974 | — | — | 218.15 | 0.8478 | 0.1522 | 0.1530 | 0.8470 | Vol. Est. |
| 11.77396616 | — | — | 218.15 | 0.8108 | 0.1892 | 0.1700 | 0.8300 | Vol. Est. |
| 13.1621188 | — | — | 218.15 | 0.7820 | 0.2180 | 0.1850 | 0.8150 | Vol. Est. |
| 13.1519863 | — | — | 218.15 | 0.7818 | 0.2182 | 0.1870 | 0.8130 | Vol. Est. |

Data summarised from TABLE 2 of Zenner63 [103]

7.1.2 Carbon Dioxide–Nitrogen Density Data

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 20.474 | 0.000105661 | 323.09 | 0.5272 | 0.4728 | Yes |
| 15.179 | 0.000143811 | 323.09 | 0.5272 | 0.4728 | Yes |
| 11.500 | 0.000195681 | 323.09 | 0.5272 | 0.4728 | Yes |
| 8.743 | 0.000266328 | 323.09 | 0.5272 | 0.4728 | Yes |
| 6.625 | 0.00036242 | 323.09 | 0.5272 | 0.4728 | Yes |
| 4.994 | 0.000493209 | 323.09 | 0.5272 | 0.4728 | Yes |
| 3.748 | 0.000671293 | 323.09 | 0.5272 | 0.4728 | Yes |
| 2.801 | 0.000913406 | 323.09 | 0.5272 | 0.4728 | Yes |
| 2.087 | 0.001242889 | 323.09 | 0.5272 | 0.4728 | Yes |
| 1.547 | 0.001692017 | 323.09 | 0.5272 | 0.4728 | Yes |
| 1.144 | 0.002303096 | 323.09 | 0.5272 | 0.4728 | Yes |
| 0.845 | 0.003132344 | 323.09 | 0.5272 | 0.4728 | Yes |
| 0.623 | 0.004266203 | 323.09 | 0.5272 | 0.4728 | Yes |
| 0.459 | 0.005808069 | 323.09 | 0.5272 | 0.4728 | Yes |
| 0.338 | 0.007903979 | 323.09 | 0.5272 | 0.4728 | Yes |
| 20.329 | 7.94959E-05 | 323.14 | 0.7650 | 0.2350 | Yes |
| 15.134 | 0.000109625 | 323.14 | 0.7650 | 0.2350 | Yes |
| 12.065 | 0.000147219 | 323.14 | 0.7650 | 0.2350 | Yes |
| 9.685 | 0.000200347 | 323.14 | 0.7650 | 0.2350 | Yes |
| 7.680 | 0.000272627 | 323.14 | 0.7650 | 0.2350 | Yes |
| 5.999 | 0.000384491 | 323.14 | 0.7650 | 0.2350 | Yes |
| 4.621 | 0.000504962 | 323.14 | 0.7650 | 0.2350 | Yes |
| 3.519 | 0.000687145 | 323.14 | 0.7650 | 0.2350 | Yes |
| 2.657 | 0.000935049 | 323.14 | 0.7650 | 0.2350 | Yes |
| 1.996 | 0.00127243 | 323.14 | 0.7650 | 0.2350 | Yes |
| 1.486 | 0.001732275 | 323.14 | 0.7650 | 0.2350 | Yes |
| 1.104 | 0.002356004 | 323.14 | 0.7650 | 0.2350 | Yes |
| 0.819 | 0.003206696 | 323.14 | 0.7650 | 0.2350 | Yes |
| 0.606 | 0.004363506 | 323.14 | 0.7650 | 0.2350 | Yes |
| 0.448 | 0.005935406 | 323.14 | 0.7650 | 0.2350 | Yes |
| 20.332 | 0.000130918 | 323.15 | 0.2150 | 0.7850 | Yes |
| 14.677 | 0.000178175 | 323.15 | 0.2150 | 0.7850 | Yes |
| 10.766 | 0.000242253 | 323.15 | 0.2150 | 0.7850 | Yes |
| 7.924 | 0.000329986 | 323.15 | 0.2150 | 0.7850 | Yes |
| 5.851 | 0.000449058 | 323.15 | 0.2150 | 0.7850 | Yes |
| 4.320 | 0.000611002 | 323.15 | 0.2150 | 0.7850 | Yes |
| 3.188 | 0.000831498 | 323.15 | 0.2150 | 0.7850 | Yes |
| 2.350 | 0.001131779 | 323.15 | 0.2150 | 0.7850 | Yes |
| 1.731 | 0.00154038 | 323.15 | 0.2150 | 0.7850 | Yes |
| 1.275 | 0.002095508 | 323.15 | 0.2150 | 0.7850 | Yes |
| 0.938 | 0.002940945 | 333.15 | 0.2150 | 0.7850 | Yes |
| 0.690 | 0.004002396 | 333.15 | 0.2150 | 0.7850 | Yes |
| 0.508 | 0.005440687 | 333.15 | 0.2150 | 0.7850 | Yes |
| 0.373 | 0.007415778 | 333.15 | 0.2150 | 0.7850 | Yes |
| 20.164 | 0.000117947 | 333.15 | 0.4565 | 0.5435 | Yes |
| 14.929 | 0.000160513 | 333.15 | 0.4565 | 0.5435 | Yes |
| 11.222 | 0.000218447 | 333.15 | 0.4565 | 0.5435 | Yes |
| 8.456 | 0.000297306 | 333.15 | 0.4565 | 0.5435 | Yes |
| 6.356 | 0.000404556 | 333.15 | 0.4565 | 0.5435 | Yes |
| 4.758 | 0.000550558 | 333.15 | 0.4565 | 0.5435 | Yes |
| 3.547 | 0.000749225 | 333.15 | 0.4565 | 0.5435 | Yes |
| 2.635 | 0.001019578 | 333.15 | 0.4565 | 0.5435 | Yes |
| 1.952 | 0.001387536 | 333.15 | 0.4565 | 0.5435 | Yes |
| 1.443 | 0.001888297 | 333.15 | 0.4565 | 0.5435 | Yes |
| 1.065 | 0.002569173 | 333.15 | 0.4565 | 0.5435 | Yes |
| 0.785 | 0.003496505 | 333.15 | 0.4565 | 0.5435 | Yes |
| 0.578 | 0.004759257 | 333.15 | 0.4565 | 0.5435 | Yes |
| 0.425 | 0.006481714 | 333.15 | 0.4565 | 0.5435 | Yes |
| 4.872 | 0.000508213 | 333.18 | 0.6925 | 0.3075 | Yes |
| 3.771 | 0.000674078 | 333.18 | 0.6925 | 0.3075 | Yes |
| 2.838 | 0.000917157 | 333.18 | 0.6925 | 0.3075 | Yes |
| 2.122 | 0.001248162 | 333.18 | 0.6925 | 0.3075 | Yes |
| 1.579 | 0.001698795 | 333.18 | 0.6925 | 0.3075 | Yes |
| 1.170 | 0.002312062 | 333.18 | 0.6925 | 0.3075 | Yes |
| 0.865 | 0.003147474 | 333.18 | 0.6925 | 0.3075 | Yes |
| 0.639 | 0.004280607 | 333.18 | 0.6925 | 0.3075 | Yes |
| 0.471 | 0.005827445 | 333.18 | 0.6925 | 0.3075 | Yes |
| 0.347 | 0.007925841 | 333.18 | 0.6925 | 0.3075 | Yes |
| 20.110 | 0.000140412 | 343.11 | 0.2510 | 0.7490 | Yes |
| 14.537 | 0.000191081 | 343.11 | 0.2510 | 0.7490 | Yes |
| 10.647 | 0.000260064 | 343.11 | 0.2510 | 0.7490 | Yes |
| 7.844 | 0.000353906 | 343.11 | 0.2510 | 0.7490 | Yes |
| 5.787 | 0.000481575 | 343.11 | 0.2510 | 0.7490 | Yes |
| 4.270 | 0.00065547 | 343.11 | 0.2510 | 0.7490 | Yes |
| 3.149 | 0.000891979 | 343.11 | 0.2510 | 0.7490 | Yes |
| 2.320 | 0.001214028 | 343.11 | 0.2510 | 0.7490 | Yes |
| 1.710 | 0.00165144 | 343.11 | 0.2510 | 0.7490 | Yes |
| 1.258 | 0.002248658 | 343.11 | 0.2510 | 0.7490 | Yes |
| 0.926 | 0.003059802 | 343.11 | 0.2510 | 0.7490 | Yes |
| 0.682 | 0.004159948 | 343.11 | 0.2510 | 0.7490 | Yes |
| 0.501 | 0.005670816 | 343.11 | 0.2510 | 0.7490 | Yes |

Data summarised from Table 1 of Altunin72 [118]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 20.072 | 0.000123665 | 343.11 | 0.4738 | 0.5262 | Yes |
| 14.857 | 0.000168302 | 343.11 | 0.4738 | 0.5262 | Yes |
| 11.149 | 0.000229061 | 343.11 | 0.4738 | 0.5262 | Yes |
| 8.384 | 0.000311716 | 343.11 | 0.4738 | 0.5262 | Yes |
| 6.289 | 0.000424174 | 343.11 | 0.4738 | 0.5262 | Yes |
| 4.699 | 0.000577294 | 343.11 | 0.4738 | 0.5262 | Yes |
| 3.498 | 0.000785614 | 343.11 | 0.4738 | 0.5262 | Yes |
| 2.596 | 0.001069021 | 343.11 | 0.4738 | 0.5262 | Yes |
| 1.922 | 0.001453847 | 343.11 | 0.4738 | 0.5262 | Yes |
| 1.419 | 0.001980658 | 343.11 | 0.4738 | 0.5262 | Yes |
| 1.047 | 0.002692289 | 343.11 | 0.4738 | 0.5262 | Yes |
| 0.772 | 0.003665742 | 343.11 | 0.4738 | 0.5262 | Yes |
| 0.568 | 0.004992356 | 343.11 | 0.4738 | 0.5262 | Yes |
| 0.418 | 0.006793427 | 343.11 | 0.4738 | 0.5262 | Yes |
| 20.072 | 9.70586E-05 | 343.11 | 0.7195 | 0.2805 | Yes |
| 15.335 | 0.0001321 | 343.11 | 0.7195 | 0.2805 | Yes |
| 12.011 | 0.000179774 | 343.11 | 0.7195 | 0.2805 | Yes |
| 9.403 | 0.000244654 | 343.11 | 0.7195 | 0.2805 | Yes |
| 7.286 | 0.00033285 | 343.11 | 0.7195 | 0.2805 | Yes |
| 5.585 | 0.000453073 | 343.11 | 0.7195 | 0.2805 | Yes |
| 4.236 | 0.000616754 | 343.11 | 0.7195 | 0.2805 | Yes |
| 3.188 | 0.000839099 | 343.11 | 0.7195 | 0.2805 | Yes |
| 2.384 | 0.001142067 | 343.11 | 0.7195 | 0.2805 | Yes |
| 1.774 | 0.001554232 | 343.11 | 0.7195 | 0.2805 | Yes |
| 1.316 | 0.002114435 | 343.11 | 0.7195 | 0.2805 | Yes |
| 0.973 | 0.002877799 | 343.11 | 0.7195 | 0.2805 | Yes |
| 0.718 | 0.003918791 | 343.11 | 0.7195 | 0.2805 | Yes |
| 0.529 | 0.005339381 | 343.11 | 0.7195 | 0.2805 | Yes |
| 0.390 | 0.007252632 | 343.11 | 0.7195 | 0.2805 | Yes |

Continued: Data summarised from Table 1 of Altunin72 [118]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|------------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 2.4115350 | 0.000754 | 273.15 | 1.000 | 0.000 | Yes |
| 2.5837875 | 0.000692 | 273.15 | 1.000 | 0.000 | Yes |
| 2.9688225 | 0.000573 | 273.15 | 1.000 | 0.000 | Yes |
| 3.1613400 | 0.000522 | 273.15 | 1.000 | 0.000 | Yes |
| 3.3538575 | 0.000476 | 273.15 | 1.000 | 0.000 | Yes |
| 4.9041300 | 0.0000451 | 273.15 | 1.000 | 0.000 | Yes |
| 7.4980500 | 0.0000442 | 273.15 | 1.000 | 0.000 | Yes |
| 9.0584550 | 0.0000438 | 273.15 | 1.000 | 0.000 | Yes |
| 11.3787975 | 0.0000431 | 273.15 | 1.000 | 0.000 | Yes |
| 12.1590000 | 0.0000425 | 273.15 | 1.000 | 0.000 | Yes |
| 14.5097400 | 0.000042 | 273.15 | 1.000 | 0.000 | Yes |
| 7.4980500 | 0.0000483 | 273.15 | 0.929 | 0.071 | Yes |
| 9.0584550 | 0.0000471 | 273.15 | 0.929 | 0.071 | Yes |
| 11.3889300 | 0.0000463 | 273.15 | 0.929 | 0.071 | Yes |
| 12.1691325 | 0.0000457 | 273.15 | 0.929 | 0.071 | Yes |
| 12.9493350 | 0.0000454 | 273.15 | 0.929 | 0.071 | Yes |
| 14.5097400 | 0.0000445 | 273.15 | 0.929 | 0.071 | Yes |
| 9.8386575 | 0.0000511 | 273.15 | 0.872 | 0.128 | Yes |
| 10.2338250 | 0.0000506 | 273.15 | 0.872 | 0.128 | Yes |
| 10.6087275 | 0.0000504 | 273.15 | 0.872 | 0.128 | Yes |
| 11.3889300 | 0.0000498 | 273.15 | 0.872 | 0.128 | Yes |
| 12.5541675 | 0.0000489 | 273.15 | 0.872 | 0.128 | Yes |
| 14.5097400 | 0.0000472 | 273.15 | 0.872 | 0.128 | Yes |
| 2.4216675 | 0.000811 | 273.15 | 0.786 | 0.214 | Yes |
| 2.9789550 | 0.000635 | 273.15 | 0.786 | 0.214 | Yes |
| 3.3639900 | 0.000545 | 273.15 | 0.786 | 0.214 | Yes |
| 4.1340600 | 0.000414 | 273.15 | 0.786 | 0.214 | Yes |
| 4.9142625 | 0.000321 | 273.15 | 0.786 | 0.214 | Yes |
| 12.0171450 | 0.000066 | 273.15 | 0.746 | 0.254 | Yes |
| 12.1691325 | 0.000065 | 273.15 | 0.746 | 0.254 | Yes |
| 12.9493350 | 0.0000622 | 273.15 | 0.746 | 0.254 | Yes |
| 13.7295375 | 0.0000587 | 273.15 | 0.746 | 0.254 | Yes |
| 14.5097400 | 0.0000585 | 273.15 | 0.746 | 0.254 | Yes |
| 2.4216675 | 0.000827 | 273.15 | 0.702 | 0.298 | Yes |
| 3.3639900 | 0.000565 | 273.15 | 0.702 | 0.298 | Yes |
| 4.1441925 | 0.000437 | 273.15 | 0.702 | 0.298 | Yes |
| 4.9243950 | 0.000348 | 273.15 | 0.702 | 0.298 | Yes |
| 5.6944650 | 0.000281 | 273.15 | 0.702 | 0.298 | Yes |
| 6.2416200 | 0.000244 | 273.15 | 0.702 | 0.298 | Yes |
| 6.4746675 | 0.000227 | 273.15 | 0.702 | 0.298 | Yes |
| 12.0171450 | 0.0000791 | 273.15 | 0.694 | 0.306 | Yes |
| 12.1691325 | 0.0000783 | 273.15 | 0.694 | 0.306 | Yes |
| 12.9493350 | 0.0000731 | 273.15 | 0.694 | 0.306 | Yes |
| 13.7295375 | 0.0000696 | 273.15 | 0.694 | 0.306 | Yes |
| 14.5097400 | 0.0000667 | 273.15 | 0.694 | 0.306 | Yes |
| 11.3889300 | 0.000102 | 273.15 | 0.633 | 0.367 | Yes |
| 12.1691325 | 0.0000937 | 273.15 | 0.633 | 0.367 | Yes |
| 12.9594675 | 0.000087 | 273.15 | 0.633 | 0.367 | Yes |
| 13.7396700 | 0.0000812 | 273.15 | 0.633 | 0.367 | Yes |
| 14.5198725 | 0.0000773 | 273.15 | 0.633 | 0.367 | Yes |

Data summarised from Table 2 and 4 of Arai71 [53]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | Usable Data Point? |
|------------|--------------------------------------|---------------|-------------------|------------------|--------------------|
| 2.6749800 | 0.000756 | 273.15 | 0.626 | 0.374 | Yes |
| 3.3639900 | 0.000579 | 273.15 | 0.626 | 0.374 | Yes |
| 4.1441925 | 0.000453 | 273.15 | 0.626 | 0.374 | Yes |
| 4.9142625 | 0.000366 | 273.15 | 0.626 | 0.374 | Yes |
| 6.7178475 | 0.000239 | 273.15 | 0.626 | 0.374 | Yes |
| 7.4980500 | 0.000203 | 273.15 | 0.626 | 0.374 | Yes |
| 8.6734200 | 0.00016 | 273.15 | 0.626 | 0.374 | Yes |
| 9.0584550 | 0.000149 | 273.15 | 0.626 | 0.374 | Yes |
| 2.9890875 | 0.000675 | 273.15 | 0.576 | 0.424 | Yes |
| 3.3741225 | 0.000587 | 273.15 | 0.576 | 0.424 | Yes |
| 4.1441925 | 0.000462 | 273.15 | 0.576 | 0.424 | Yes |
| 4.9243950 | 0.000376 | 273.15 | 0.576 | 0.424 | Yes |
| 6.7279800 | 0.000251 | 273.15 | 0.576 | 0.424 | Yes |
| 8.6734200 | 0.000175 | 273.15 | 0.576 | 0.424 | Yes |
| 10.6087275 | 0.000129 | 273.15 | 0.576 | 0.424 | Yes |
| 12.1691325 | 0.000106 | 273.15 | 0.576 | 0.424 | Yes |
| 12.9493350 | 0.000098 | 273.15 | 0.576 | 0.424 | Yes |
| 2.4318000 | 0.000869 | 273.15 | 0.492 | 0.508 | Yes |
| 3.3639900 | 0.000607 | 273.15 | 0.492 | 0.508 | Yes |
| 4.1441925 | 0.000481 | 273.15 | 0.492 | 0.508 | Yes |
| 4.9243950 | 0.000395 | 273.15 | 0.492 | 0.508 | Yes |
| 6.7279800 | 0.00027 | 273.15 | 0.492 | 0.508 | Yes |
| 8.6734200 | 0.000195 | 273.15 | 0.492 | 0.508 | Yes |
| 10.6087275 | 0.000151 | 273.15 | 0.492 | 0.508 | Yes |
| 11.3889300 | 0.000138 | 273.15 | 0.492 | 0.508 | Yes |
| 12.9493350 | 0.000117 | 273.15 | 0.492 | 0.508 | Yes |
| 14.5097400 | 0.000102 | 273.15 | 0.492 | 0.508 | Yes |
| 2.4318000 | 0.000821 | 288.15 | 1.000 | 0.000 | Yes |
| 2.9890875 | 0.000634 | 288.15 | 1.000 | 0.000 | Yes |
| 3.7692900 | 0.000461 | 288.15 | 1.000 | 0.000 | Yes |
| 4.3873725 | 0.000361 | 288.15 | 1.000 | 0.000 | Yes |
| 4.5596250 | 0.000344 | 288.15 | 1.000 | 0.000 | Yes |
| 4.7217450 | 0.000323 | 288.15 | 1.000 | 0.000 | Yes |
| 4.8737325 | 0.000302 | 288.15 | 1.000 | 0.000 | Yes |
| 4.9243950 | 0.000288 | 288.15 | 1.000 | 0.000 | Yes |
| 5.4208875 | 0.0000525 | 288.15 | 1.000 | 0.000 | Yes |
| 6.7279800 | 0.000051 | 288.15 | 1.000 | 0.000 | Yes |
| 10.6188600 | 0.0000486 | 288.15 | 1.000 | 0.000 | Yes |
| 12.1792650 | 0.0000478 | 288.15 | 1.000 | 0.000 | Yes |
| 14.5198725 | 0.0000468 | 288.15 | 1.000 | 0.000 | Yes |
| 8.2579875 | 0.0000552 | 288.15 | 0.940 | 0.060 | Yes |
| 9.0685875 | 0.0000538 | 288.15 | 0.940 | 0.060 | Yes |
| 9.8386575 | 0.0000527 | 288.15 | 0.940 | 0.060 | Yes |
| 10.6188600 | 0.0000517 | 288.15 | 0.940 | 0.060 | Yes |
| 11.7840975 | 0.0000507 | 288.15 | 0.940 | 0.060 | Yes |
| 13.3445025 | 0.0000496 | 288.15 | 0.940 | 0.060 | Yes |
| 13.7396700 | 0.0000492 | 288.15 | 0.940 | 0.060 | Yes |
| 2.4318000 | 0.000838 | 288.15 | 0.918 | 0.082 | Yes |
| 2.9890875 | 0.000653 | 288.15 | 0.918 | 0.082 | Yes |
| 3.7692900 | 0.000485 | 288.15 | 0.918 | 0.082 | Yes |
| 4.5393600 | 0.00037 | 288.15 | 0.918 | 0.082 | Yes |
| 5.9984400 | 0.000221 | 288.15 | 0.918 | 0.082 | Yes |
| 2.4419325 | 0.00085 | 288.15 | 0.897 | 0.103 | Yes |
| 3.7692900 | 0.000495 | 288.15 | 0.897 | 0.103 | Yes |
| 4.9345275 | 0.000335 | 288.15 | 0.897 | 0.103 | Yes |
| 5.7147300 | 0.000259 | 288.15 | 0.897 | 0.103 | Yes |
| 9.4637550 | 0.0000606 | 288.15 | 0.897 | 0.103 | Yes |
| 9.8589225 | 0.0000593 | 288.15 | 0.897 | 0.103 | Yes |
| 10.2439575 | 0.000058 | 288.15 | 0.897 | 0.103 | Yes |
| 10.6188600 | 0.0000572 | 288.15 | 0.897 | 0.103 | Yes |
| 12.1792650 | 0.0000544 | 288.15 | 0.897 | 0.103 | Yes |
| 13.7396700 | 0.0000526 | 288.15 | 0.897 | 0.103 | Yes |
| 14.5198725 | 0.0000518 | 288.15 | 0.897 | 0.103 | Yes |
| 9.8589225 | 0.000068 | 288.15 | 0.868 | 0.132 | Yes |
| 10.2439575 | 0.0000654 | 288.15 | 0.868 | 0.132 | Yes |
| 10.6188600 | 0.0000634 | 288.15 | 0.868 | 0.132 | Yes |
| 11.3990625 | 0.0000605 | 288.15 | 0.868 | 0.132 | Yes |
| 12.1792650 | 0.0000586 | 288.15 | 0.868 | 0.132 | Yes |
| 13.3546350 | 0.0000563 | 288.15 | 0.868 | 0.132 | Yes |
| 14.5198725 | 0.0000547 | 288.15 | 0.868 | 0.132 | Yes |
| 10.0919700 | 0.0000744 | 288.15 | 0.845 | 0.155 | Yes |
| 10.2439575 | 0.0000729 | 288.15 | 0.845 | 0.155 | Yes |
| 10.6188600 | 0.0000696 | 288.15 | 0.845 | 0.155 | Yes |
| 11.3990625 | 0.0000659 | 288.15 | 0.845 | 0.155 | Yes |
| 10.6188600 | 0.0000757 | 288.15 | 0.827 | 0.173 | Yes |
| 11.3990625 | 0.0000697 | 288.15 | 0.827 | 0.173 | Yes |
| 12.1792650 | 0.0000656 | 288.15 | 0.827 | 0.173 | Yes |
| 12.9594675 | 0.000062 | 288.15 | 0.827 | 0.173 | Yes |
| 13.7396700 | 0.0000604 | 288.15 | 0.827 | 0.173 | Yes |
| 2.4419325 | 0.000869 | 288.15 | 0.813 | 0.187 | Yes |
| 4.9345275 | 0.000362 | 288.15 | 0.813 | 0.187 | Yes |
| 6.7381125 | 0.00022 | 288.15 | 0.813 | 0.187 | Yes |
| 7.5183150 | 0.000177 | 288.15 | 0.813 | 0.187 | Yes |
| 10.1426325 | 0.0000861 | 288.15 | 0.812 | 0.188 | Yes |
| 10.4567400 | 0.0000819 | 288.15 | 0.812 | 0.188 | Yes |
| 11.2977375 | 0.0000743 | 288.15 | 0.812 | 0.188 | Yes |

Continued: Data summarised from Table 2 and 4 of Arai71 [53]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|------------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 12.0779400 | 0.0000691 | 288.15 | 0.812 | 0.188 | Yes |
| 12.8581425 | 0.0000657 | 288.15 | 0.812 | 0.188 | Yes |
| 13.6383450 | 0.0000629 | 288.15 | 0.812 | 0.188 | Yes |
| 9.8589225 | 0.0000978 | 288.15 | 0.801 | 0.199 | Yes |
| 10.2540900 | 0.0000909 | 288.15 | 0.801 | 0.199 | Yes |
| 10.6188600 | 0.0000855 | 288.15 | 0.801 | 0.199 | Yes |
| 11.3585325 | 0.0000773 | 288.15 | 0.801 | 0.199 | Yes |
| 12.1792650 | 0.0000716 | 288.15 | 0.801 | 0.199 | Yes |
| 13.3546350 | 0.0000661 | 288.15 | 0.801 | 0.199 | Yes |
| 14.5198725 | 0.0000625 | 288.15 | 0.801 | 0.199 | Yes |
| 2.6141850 | 0.000816 | 288.15 | 0.736 | 0.264 | Yes |
| 4.9345275 | 0.000379 | 288.15 | 0.736 | 0.264 | Yes |
| 6.7381125 | 0.000245 | 288.15 | 0.736 | 0.264 | Yes |
| 8.6835525 | 0.00016 | 288.15 | 0.736 | 0.264 | Yes |
| 10.6188600 | 0.00011 | 288.15 | 0.736 | 0.264 | Yes |
| 12.5643000 | 0.0000848 | 288.15 | 0.736 | 0.264 | Yes |
| 14.5198725 | 0.0000722 | 288.15 | 0.736 | 0.264 | Yes |
| 2.7661725 | 0.000769 | 288.15 | 0.702 | 0.298 | Yes |
| 5.0966475 | 0.000371 | 288.15 | 0.702 | 0.298 | Yes |
| 6.7381125 | 0.000253 | 288.15 | 0.702 | 0.298 | Yes |
| 10.6188600 | 0.000121 | 288.15 | 0.702 | 0.298 | Yes |
| 14.5198725 | 0.0000785 | 288.15 | 0.702 | 0.298 | Yes |

Continued: Data summarised from Table 2 and 4 of Arai71 [53]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 41.00439 | 6.06487E-05 | 300.019 | 0.447 | 0.553 | Yes |
| 38.54936 | 6.18204E-05 | 300.132 | 0.447 | 0.553 | Yes |
| 27.63501 | 7.61707E-05 | 300.030 | 0.447 | 0.553 | Yes |
| 21.86764 | 9.12959E-05 | 300.023 | 0.447 | 0.553 | Yes |
| 21.09454 | 9.31159E-05 | 299.992 | 0.447 | 0.553 | Yes |
| 17.16298 | 0.000114686 | 300.000 | 0.447 | 0.553 | Yes |
| 15.50388 | 0.000127456 | 300.006 | 0.447 | 0.553 | Yes |
| 14.46641 | 0.000137469 | 300.014 | 0.447 | 0.553 | Yes |
| 14.06685 | 0.000140289 | 299.978 | 0.447 | 0.553 | Yes |
| 11.80328 | 0.000172697 | 300.013 | 0.447 | 0.553 | Yes |
| 10.75626 | 0.000191912 | 299.975 | 0.447 | 0.553 | Yes |
| 10.07421 | 0.00020701 | 300.025 | 0.447 | 0.553 | Yes |
| 9.82850 | 0.000211375 | 299.978 | 0.447 | 0.553 | Yes |
| 8.25051 | 0.000260064 | 300.011 | 0.447 | 0.553 | Yes |
| 7.51655 | 0.00028897 | 300.000 | 0.447 | 0.553 | Yes |
| 7.02829 | 0.00031174 | 300.018 | 0.447 | 0.553 | Yes |
| 6.86538 | 0.000318493 | 299.919 | 0.447 | 0.553 | Yes |
| 5.72708 | 0.000391642 | 300.027 | 0.447 | 0.553 | Yes |
| 5.20380 | 0.0004351 | 299.999 | 0.447 | 0.553 | Yes |
| 4.85458 | 0.000469473 | 300.024 | 0.447 | 0.553 | Yes |
| 4.74645 | 0.000479904 | 299.983 | 0.447 | 0.553 | Yes |
| 3.93098 | 0.00058981 | 300.024 | 0.447 | 0.553 | Yes |
| 3.56291 | 0.000655128 | 299.984 | 0.447 | 0.553 | Yes |
| 3.31707 | 0.000707024 | 300.020 | 0.447 | 0.553 | Yes |
| 3.24311 | 0.000723134 | 299.914 | 0.447 | 0.553 | Yes |
| 2.91424 | 0.000810806 | 299.999 | 0.447 | 0.553 | Yes |
| 2.67210 | 0.000888265 | 299.995 | 0.447 | 0.553 | Yes |
| 2.41732 | 0.000986563 | 299.990 | 0.447 | 0.553 | Yes |
| 2.19764 | 0.001089645 | 299.970 | 0.447 | 0.553 | Yes |
| 1.95959 | 0.00120636 | 300.010 | 0.447 | 0.553 | Yes |
| 1.80350 | 0.001337739 | 300.005 | 0.447 | 0.553 | Yes |
| 1.62900 | 0.001485685 | 299.988 | 0.447 | 0.553 | Yes |
| 1.51258 | 0.001603618 | 300.016 | 0.447 | 0.553 | Yes |
| 1.47509 | 0.001641928 | 299.998 | 0.447 | 0.553 | Yes |
| 1.32364 | 0.001839013 | 300.008 | 0.447 | 0.553 | Yes |
| 1.21087 | 0.002014707 | 300.026 | 0.447 | 0.553 | Yes |
| 1.09235 | 0.002237737 | 299.976 | 0.447 | 0.553 | Yes |
| 1.01292 | 0.002415109 | 299.809 | 0.447 | 0.553 | Yes |
| 0.98849 | 0.002474206 | 299.977 | 0.447 | 0.553 | Yes |
| 0.88603 | 0.002769623 | 300.009 | 0.447 | 0.553 | Yes |
| 0.80990 | 0.003034257 | 300.026 | 0.447 | 0.553 | Yes |
| 0.67763 | 0.003637289 | 300.160 | 0.447 | 0.553 | Yes |
| 0.66029 | 0.003728283 | 299.978 | 0.447 | 0.553 | Yes |
| 0.59158 | 0.004171185 | 300.011 | 0.447 | 0.553 | Yes |
| 0.54047 | 0.004569757 | 300.017 | 0.447 | 0.553 | Yes |
| 0.45180 | 0.005477951 | 300.155 | 0.447 | 0.553 | Yes |
| 0.44023 | 0.005617978 | 299.985 | 0.447 | 0.553 | Yes |
| 0.39416 | 0.006282196 | 300.005 | 0.447 | 0.553 | Yes |
| 0.36004 | 0.006882312 | 300.017 | 0.447 | 0.553 | Yes |
| 0.30090 | 0.008250144 | 300.149 | 0.447 | 0.553 | Yes |
| 0.29313 | 0.008465967 | 299.991 | 0.447 | 0.553 | Yes |
| 0.26238 | 0.009460738 | 300.003 | 0.447 | 0.553 | Yes |
| 0.23963 | 0.010364842 | 300.019 | 0.447 | 0.553 | Yes |
| 0.20011 | 0.012425447 | 300.148 | 0.447 | 0.553 | Yes |
| 0.19507 | 0.012756729 | 299.997 | 0.447 | 0.553 | Yes |
| 0.17449 | 0.014249074 | 300.011 | 0.447 | 0.553 | Yes |
| 0.15934 | 0.015610365 | 300.010 | 0.447 | 0.553 | Yes |
| 0.13301 | 0.018712575 | 300.145 | 0.447 | 0.553 | Yes |
| 0.12961 | 0.019223376 | 300.006 | 0.447 | 0.553 | Yes |
| 0.11596 | 0.021459227 | 300.013 | 0.447 | 0.553 | Yes |
| 0.10590 | 0.023512814 | 300.011 | 0.447 | 0.553 | Yes |
| 0.08840 | 0.028184893 | 300.145 | 0.447 | 0.553 | Yes |

Data summarised from Table VIII of Bailey89 [82]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 9.27379 | 0.0002622 | 300 | 0.10560 | 0.89440 | Yes |
| 7.83286 | 0.0003107 | 300 | 0.10560 | 0.89440 | Yes |
| 6.14139 | 0.0003973 | 300 | 0.10560 | 0.89440 | Yes |
| 5.19435 | 0.0004707 | 300 | 0.10560 | 0.89440 | Yes |
| 4.07540 | 0.0006018 | 300 | 0.10560 | 0.89440 | Yes |
| 3.44681 | 0.0007130 | 300 | 0.10560 | 0.89440 | Yes |
| 2.70338 | 0.0009115 | 300 | 0.10560 | 0.89440 | Yes |
| 2.28539 | 0.0010800 | 300 | 0.10560 | 0.89440 | Yes |
| 1.79084 | 0.0013811 | 300 | 0.10560 | 0.89440 | Yes |
| 1.51331 | 0.0016363 | 300 | 0.10560 | 0.89440 | Yes |
| 1.18531 | 0.0020922 | 300 | 0.10560 | 0.89440 | Yes |
| 1.00124 | 0.0024789 | 300 | 0.10560 | 0.89440 | Yes |
| 0.78389 | 0.0031695 | 300 | 0.10560 | 0.89440 | Yes |
| 0.66198 | 0.0037554 | 300 | 0.10560 | 0.89440 | Yes |
| 0.51809 | 0.0048017 | 300 | 0.10560 | 0.89440 | Yes |
| 0.43745 | 0.0056890 | 300 | 0.10560 | 0.89440 | Yes |
| 0.34229 | 0.0072741 | 300 | 0.10560 | 0.89440 | Yes |
| 0.28896 | 0.0086188 | 300 | 0.10560 | 0.89440 | Yes |
| 0.22607 | 0.0110198 | 300 | 0.10560 | 0.89440 | Yes |
| 9.86634 | 0.000234078 | 300 | 0.25147 | 0.74853 | Yes |
| 8.42048 | 0.000276255 | 300 | 0.25147 | 0.74853 | Yes |
| 6.63406 | 0.00035458 | 300 | 0.25147 | 0.74853 | Yes |
| 5.66125 | 0.000418444 | 300 | 0.25147 | 0.74853 | Yes |
| 4.45281 | 0.000537127 | 300 | 0.25147 | 0.74853 | Yes |
| 3.79423 | 0.00063392 | 300 | 0.25147 | 0.74853 | Yes |
| 2.97716 | 0.000813768 | 300 | 0.25147 | 0.74853 | Yes |
| 2.53320 | 0.000960333 | 300 | 0.25147 | 0.74853 | Yes |
| 1.98351 | 0.001232833 | 300 | 0.25147 | 0.74853 | Yes |
| 1.68560 | 0.001454904 | 300 | 0.25147 | 0.74853 | Yes |
| 1.31779 | 0.001867703 | 300 | 0.25147 | 0.74853 | Yes |
| 1.11883 | 0.002204166 | 300 | 0.25147 | 0.74853 | Yes |
| 0.87366 | 0.002829597 | 300 | 0.25147 | 0.74853 | Yes |
| 0.74129 | 0.0033393 | 300 | 0.25147 | 0.74853 | Yes |
| 0.57839 | 0.004286794 | 300 | 0.25147 | 0.74853 | Yes |
| 0.49054 | 0.005059051 | 300 | 0.25147 | 0.74853 | Yes |
| 0.38254 | 0.006494403 | 300 | 0.25147 | 0.74853 | Yes |
| 0.32434 | 0.007664304 | 300 | 0.25147 | 0.74853 | Yes |
| 0.25283 | 0.009839264 | 300 | 0.25147 | 0.74853 | Yes |
| 0.21432 | 0.011611728 | 300 | 0.25147 | 0.74853 | Yes |
| 9.53694 | 0.000212203 | 300 | 0.50365 | 0.49635 | Yes |
| 8.64623 | 0.000238431 | 300 | 0.50365 | 0.49635 | Yes |
| 6.69079 | 0.000321595 | 300 | 0.50365 | 0.49635 | Yes |
| 6.04314 | 0.000361286 | 300 | 0.50365 | 0.49635 | Yes |
| 4.62709 | 0.000487176 | 300 | 0.50365 | 0.49635 | Yes |
| 4.16204 | 0.000547312 | 300 | 0.50365 | 0.49635 | Yes |
| 3.15653 | 0.00073807 | 300 | 0.50365 | 0.49635 | Yes |
| 2.83087 | 0.000828953 | 300 | 0.50365 | 0.49635 | Yes |
| 2.13134 | 0.00111809 | 300 | 0.50365 | 0.49635 | Yes |
| 1.90686 | 0.001255837 | 300 | 0.50365 | 0.49635 | Yes |
| 1.42852 | 0.001693842 | 300 | 0.50365 | 0.49635 | Yes |
| 1.27583 | 0.001902764 | 300 | 0.50365 | 0.49635 | Yes |
| 0.95265 | 0.002566058 | 300 | 0.50365 | 0.49635 | Yes |
| 0.84990 | 0.002882508 | 300 | 0.50365 | 0.49635 | Yes |
| 0.63313 | 0.00388734 | 300 | 0.50365 | 0.49635 | Yes |
| 0.56442 | 0.004366873 | 300 | 0.50365 | 0.49635 | Yes |
| 0.41982 | 0.00588909 | 300 | 0.50365 | 0.49635 | Yes |
| 0.37407 | 0.006615614 | 300 | 0.50365 | 0.49635 | Yes |
| 0.27794 | 0.008921975 | 300 | 0.50365 | 0.49635 | Yes |
| 0.24757 | 0.010022535 | 300 | 0.50365 | 0.49635 | Yes |
| 8.90956 | 0.000191352 | 300 | 0.71105 | 0.28895 | Yes |
| 7.95354 | 0.000225637 | 300 | 0.71105 | 0.28895 | Yes |
| 6.62487 | 0.000289938 | 300 | 0.71105 | 0.28895 | Yes |
| 5.83538 | 0.000341839 | 300 | 0.71105 | 0.28895 | Yes |
| 4.76488 | 0.00043924 | 300 | 0.71105 | 0.28895 | Yes |
| 4.14835 | 0.00051783 | 300 | 0.71105 | 0.28895 | Yes |
| 3.33496 | 0.000665497 | 300 | 0.71105 | 0.28895 | Yes |
| 2.87919 | 0.000784464 | 300 | 0.71105 | 0.28895 | Yes |
| 2.29002 | 0.001008083 | 300 | 0.71105 | 0.28895 | Yes |
| 1.96530 | 0.001188433 | 300 | 0.71105 | 0.28895 | Yes |
| 1.55174 | 0.001527188 | 300 | 0.71105 | 0.28895 | Yes |
| 1.32645 | 0.001800463 | 300 | 0.71105 | 0.28895 | Yes |
| 1.04221 | 0.002313622 | 300 | 0.71105 | 0.28895 | Yes |
| 0.88855 | 0.002727658 | 300 | 0.71105 | 0.28895 | Yes |
| 0.69589 | 0.003505079 | 300 | 0.71105 | 0.28895 | Yes |
| 0.59227 | 0.004132288 | 300 | 0.71105 | 0.28895 | Yes |
| 0.46284 | 0.005310094 | 300 | 0.71105 | 0.28895 | Yes |
| 0.39347 | 0.00626031 | 300 | 0.71105 | 0.28895 | Yes |
| 0.30704 | 0.008044892 | 300 | 0.71105 | 0.28895 | Yes |
| 0.26083 | 0.009484287 | 300 | 0.71105 | 0.28895 | Yes |

Data summarised from Table I and II of Brugge89 [85]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 5.50863 | 0.000320691 | 300 | 0.90921 | 0.09079 | Yes |
| 5.21854 | 0.000348 | 300 | 0.90921 | 0.09079 | Yes |
| 4.09677 | 0.000485818 | 300 | 0.90921 | 0.09079 | Yes |
| 3.84375 | 0.000527199 | 300 | 0.90921 | 0.09079 | Yes |
| 2.92334 | 0.000735894 | 300 | 0.90921 | 0.09079 | Yes |
| 2.72538 | 0.000798667 | 300 | 0.90921 | 0.09079 | Yes |
| 2.03001 | 0.001114977 | 300 | 0.90921 | 0.09079 | Yes |
| 1.88511 | 0.001209941 | 300 | 0.90921 | 0.09079 | Yes |
| 1.38528 | 0.001689132 | 300 | 0.90921 | 0.09079 | Yes |
| 1.28301 | 0.001832996 | 300 | 0.90921 | 0.09079 | Yes |
| 0.93460 | 0.002558914 | 300 | 0.90921 | 0.09079 | Yes |
| 0.86408 | 0.002776954 | 300 | 0.90921 | 0.09079 | Yes |
| 0.62584 | 0.003876602 | 300 | 0.90921 | 0.09079 | Yes |
| 0.57793 | 0.004207079 | 300 | 0.90921 | 0.09079 | Yes |
| 0.41703 | 0.005872872 | 300 | 0.90921 | 0.09079 | Yes |
| 0.38482 | 0.006373517 | 300 | 0.90921 | 0.09079 | Yes |
| 0.27699 | 0.008897268 | 300 | 0.90921 | 0.09079 | Yes |
| 0.25547 | 0.009655699 | 300 | 0.90921 | 0.09079 | Yes |
| 9.81270 | 0.000268453 | 320 | 0.10560 | 0.89440 | Yes |
| 8.23109 | 0.000319592 | 320 | 0.10560 | 0.89440 | Yes |
| 6.46611 | 0.000406735 | 320 | 0.10560 | 0.89440 | Yes |
| 5.43492 | 0.000484169 | 320 | 0.10560 | 0.89440 | Yes |
| 4.27577 | 0.000616159 | 320 | 0.10560 | 0.89440 | Yes |
| 3.59568 | 0.000733446 | 320 | 0.10560 | 0.89440 | Yes |
| 2.82923 | 0.000933416 | 320 | 0.10560 | 0.89440 | Yes |
| 2.37918 | 0.001111026 | 320 | 0.10560 | 0.89440 | Yes |
| 1.87154 | 0.001414031 | 320 | 0.10560 | 0.89440 | Yes |
| 1.57337 | 0.001683244 | 320 | 0.10560 | 0.89440 | Yes |
| 1.23738 | 0.002142152 | 320 | 0.10560 | 0.89440 | Yes |
| 1.04001 | 0.002550072 | 320 | 0.10560 | 0.89440 | Yes |
| 0.81772 | 0.003245337 | 320 | 0.10560 | 0.89440 | Yes |
| 0.68719 | 0.003863213 | 320 | 0.10560 | 0.89440 | Yes |
| 0.54019 | 0.004916632 | 320 | 0.10560 | 0.89440 | Yes |
| 0.45392 | 0.005852497 | 320 | 0.10560 | 0.89440 | Yes |
| 0.35678 | 0.007448273 | 320 | 0.10560 | 0.89440 | Yes |
| 0.29977 | 0.008866239 | 320 | 0.10560 | 0.89440 | Yes |
| 0.23559 | 0.011283887 | 320 | 0.10560 | 0.89440 | Yes |
| 10.59715 | 0.00023813 | 320 | 0.25147 | 0.74853 | Yes |
| 9.01444 | 0.000281026 | 320 | 0.25147 | 0.74853 | Yes |
| 7.07010 | 0.000360801 | 320 | 0.25147 | 0.74853 | Yes |
| 6.01957 | 0.000425738 | 320 | 0.25147 | 0.74853 | Yes |
| 4.71948 | 0.000546628 | 320 | 0.25147 | 0.74853 | Yes |
| 4.01581 | 0.000644936 | 320 | 0.25147 | 0.74853 | Yes |
| 3.14400 | 0.000828091 | 320 | 0.25147 | 0.74853 | Yes |
| 2.67268 | 0.000977032 | 320 | 0.25147 | 0.74853 | Yes |
| 2.08949 | 0.001254527 | 320 | 0.25147 | 0.74853 | Yes |
| 1.77468 | 0.001480173 | 320 | 0.25147 | 0.74853 | Yes |
| 1.38583 | 0.001900575 | 320 | 0.25147 | 0.74853 | Yes |
| 1.17630 | 0.002242412 | 320 | 0.25147 | 0.74853 | Yes |
| 0.91777 | 0.002879406 | 320 | 0.25147 | 0.74853 | Yes |
| 0.77864 | 0.003397259 | 320 | 0.25147 | 0.74853 | Yes |
| 0.60715 | 0.004362207 | 320 | 0.25147 | 0.74853 | Yes |
| 0.51493 | 0.005146906 | 320 | 0.25147 | 0.74853 | Yes |
| 0.34033 | 0.007797486 | 320 | 0.25147 | 0.74853 | Yes |
| 0.30137 | 0.008801516 | 320 | 0.25147 | 0.74853 | Yes |
| 0.26519 | 0.010012375 | 320 | 0.25147 | 0.74853 | Yes |
| 0.22483 | 0.01181317 | 320 | 0.25147 | 0.74853 | Yes |
| 10.20113 | 0.000222635 | 320 | 0.50365 | 0.49635 | Yes |
| 9.20586 | 0.000249926 | 320 | 0.50365 | 0.49635 | Yes |
| 7.03706 | 0.000337371 | 320 | 0.50365 | 0.49635 | Yes |
| 6.34060 | 0.000378417 | 320 | 0.50365 | 0.49635 | Yes |
| 4.80926 | 0.00051124 | 320 | 0.50365 | 0.49635 | Yes |
| 4.32407 | 0.000573058 | 320 | 0.50365 | 0.49635 | Yes |
| 3.25577 | 0.000774537 | 320 | 0.50365 | 0.49635 | Yes |
| 2.92123 | 0.000867984 | 320 | 0.50365 | 0.49635 | Yes |
| 2.18700 | 0.001173513 | 320 | 0.50365 | 0.49635 | Yes |
| 1.95904 | 0.001314915 | 320 | 0.50365 | 0.49635 | Yes |
| 1.46056 | 0.00177834 | 320 | 0.50365 | 0.49635 | Yes |
| 1.30719 | 0.001991992 | 320 | 0.50365 | 0.49635 | Yes |
| 0.97179 | 0.002694408 | 320 | 0.50365 | 0.49635 | Yes |
| 0.86918 | 0.003017791 | 320 | 0.50365 | 0.49635 | Yes |
| 0.64489 | 0.004082168 | 320 | 0.50365 | 0.49635 | Yes |
| 0.57649 | 0.00457181 | 320 | 0.50365 | 0.49635 | Yes |
| 0.42718 | 0.006184578 | 320 | 0.50365 | 0.49635 | Yes |
| 0.38174 | 0.006926234 | 320 | 0.50365 | 0.49635 | Yes |
| 0.28263 | 0.00936993 | 320 | 0.50365 | 0.49635 | Yes |
| 0.25251 | 0.010493088 | 320 | 0.50365 | 0.49635 | Yes |

Continued: Data summarised from Table I and II of Brugge89 [85]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 9.71988 | 0.000204633 | 320 | 0.71105 | 0.28895 | Yes |
| 8.25659 | 0.000252739 | 320 | 0.71105 | 0.28895 | Yes |
| 7.01148 | 0.000309987 | 320 | 0.71105 | 0.28895 | Yes |
| 5.88416 | 0.00038291 | 320 | 0.71105 | 0.28895 | Yes |
| 4.94061 | 0.000469565 | 320 | 0.71105 | 0.28895 | Yes |
| 4.10141 | 0.000580061 | 320 | 0.71105 | 0.28895 | Yes |
| 3.41246 | 0.000711332 | 320 | 0.71105 | 0.28895 | Yes |
| 2.81027 | 0.00087867 | 320 | 0.71105 | 0.28895 | Yes |
| 2.32297 | 0.001077517 | 320 | 0.71105 | 0.28895 | Yes |
| 1.90218 | 0.001331084 | 320 | 0.71105 | 0.28895 | Yes |
| 1.56509 | 0.00163249 | 320 | 0.71105 | 0.28895 | Yes |
| 1.27672 | 0.002016586 | 320 | 0.71105 | 0.28895 | Yes |
| 1.04735 | 0.002473111 | 320 | 0.71105 | 0.28895 | Yes |
| 0.85216 | 0.003055051 | 320 | 0.71105 | 0.28895 | Yes |
| 0.69765 | 0.003746606 | 320 | 0.71105 | 0.28895 | Yes |
| 0.56666 | 0.004628266 | 320 | 0.71105 | 0.28895 | Yes |
| 0.46331 | 0.005675658 | 320 | 0.71105 | 0.28895 | Yes |
| 0.37588 | 0.007011371 | 320 | 0.71105 | 0.28895 | Yes |
| 0.30705 | 0.008598182 | 320 | 0.71105 | 0.28895 | Yes |
| 0.24891 | 0.010622171 | 320 | 0.71105 | 0.28895 | Yes |
| 7.30279 | 0.000254944 | 320 | 0.90921 | 0.09079 | Yes |
| 6.52578 | 0.000300779 | 320 | 0.90921 | 0.09079 | Yes |
| 5.43121 | 0.000386191 | 320 | 0.90921 | 0.09079 | Yes |
| 4.77261 | 0.000455571 | 320 | 0.90921 | 0.09079 | Yes |
| 3.88549 | 0.000585075 | 320 | 0.90921 | 0.09079 | Yes |
| 3.37337 | 0.00069021 | 320 | 0.90921 | 0.09079 | Yes |
| 2.70577 | 0.000886289 | 320 | 0.90921 | 0.09079 | Yes |
| 2.33018 | 0.001045593 | 320 | 0.90921 | 0.09079 | Yes |
| 1.85038 | 0.001342674 | 320 | 0.90921 | 0.09079 | Yes |
| 1.58500 | 0.001583887 | 320 | 0.90921 | 0.09079 | Yes |
| 1.25019 | 0.00203411 | 320 | 0.90921 | 0.09079 | Yes |
| 1.06716 | 0.002399456 | 320 | 0.90921 | 0.09079 | Yes |
| 0.83807 | 0.003081399 | 320 | 0.90921 | 0.09079 | Yes |
| 0.71366 | 0.003635051 | 320 | 0.90921 | 0.09079 | Yes |
| 0.55886 | 0.004668018 | 320 | 0.90921 | 0.09079 | Yes |
| 0.47514 | 0.005506977 | 320 | 0.90921 | 0.09079 | Yes |
| 0.37137 | 0.007071863 | 320 | 0.90921 | 0.09079 | Yes |
| 0.31543 | 0.008342531 | 320 | 0.90921 | 0.09079 | Yes |
| 0.24622 | 0.010713609 | 320 | 0.90921 | 0.09079 | Yes |
| 0.20900 | 0.012638261 | 320 | 0.90921 | 0.09079 | Yes |

Continued: Data summarised from Table I and II of Brugge89 [85]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 68.759 | 0.0000456162759 | 225 | 0.10560 | 0.89440 | Yes |
| 62.510 | 0.0000469792352 | 225 | 0.10560 | 0.89440 | Yes |
| 57.402 | 0.0000482951801 | 225 | 0.10560 | 0.89440 | Yes |
| 51.819 | 0.0000500250125 | 225 | 0.10560 | 0.89440 | Yes |
| 45.955 | 0.0000522575251 | 225 | 0.10560 | 0.89440 | Yes |
| 40.271 | 0.0000550721445 | 225 | 0.10560 | 0.89440 | Yes |
| 34.553 | 0.0000588997526 | 225 | 0.10560 | 0.89440 | Yes |
| 28.832 | 0.0000645036445 | 225 | 0.10560 | 0.89440 | Yes |
| 23.073 | 0.0000737408746 | 225 | 0.10560 | 0.89440 | Yes |
| 17.334 | 0.0000914996798 | 225 | 0.10560 | 0.89440 | Yes |
| 11.565 | 0.0001350438893 | 225 | 0.10560 | 0.89440 | Yes |
| 5.789 | 0.0002881844380 | 225 | 0.10560 | 0.89440 | Yes |
| 68.723 | 0.0000432806752 | 225 | 0.25147 | 0.74853 | Yes |
| 63.995 | 0.0000440703363 | 225 | 0.25147 | 0.74853 | Yes |
| 59.486 | 0.0000449155587 | 225 | 0.25147 | 0.74853 | Yes |
| 54.635 | 0.0000459643317 | 225 | 0.25147 | 0.74853 | Yes |
| 50.028 | 0.0000471164719 | 225 | 0.25147 | 0.74853 | Yes |
| 45.559 | 0.0000484449181 | 225 | 0.25147 | 0.74853 | Yes |
| 40.832 | 0.0000501353655 | 225 | 0.25147 | 0.74853 | Yes |
| 36.052 | 0.0000522821143 | 225 | 0.25147 | 0.74853 | Yes |
| 31.521 | 0.0000549571334 | 225 | 0.25147 | 0.74853 | Yes |
| 26.560 | 0.0000590841950 | 225 | 0.25147 | 0.74853 | Yes |
| 22.097 | 0.0000648256191 | 225 | 0.25147 | 0.74853 | Yes |
| 17.324 | 0.0000758265089 | 225 | 0.25147 | 0.74853 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------------|-------------------|------------------|--------------------|
| 68.757 | 0.0000396589332 | 225 | 0.50365 | 0.49635 | Yes |
| 64.284 | 0.0000401026628 | 225 | 0.50365 | 0.49635 | Yes |
| 59.971 | 0.0000405695971 | 225 | 0.50365 | 0.49635 | Yes |
| 55.490 | 0.0000411048997 | 225 | 0.50365 | 0.49635 | Yes |
| 51.251 | 0.0000416736123 | 225 | 0.50365 | 0.49635 | Yes |
| 47.029 | 0.0000423047635 | 225 | 0.50365 | 0.49635 | Yes |
| 42.734 | 0.0000430366672 | 225 | 0.50365 | 0.49635 | Yes |
| 38.334 | 0.0000439039382 | 225 | 0.50365 | 0.49635 | Yes |
| 33.940 | 0.0000449337228 | 225 | 0.50365 | 0.49635 | Yes |
| 29.435 | 0.0000462384982 | 225 | 0.50365 | 0.49635 | Yes |
| 25.084 | 0.0000478858402 | 225 | 0.50365 | 0.49635 | Yes |
| 68.765 | 0.0000373203956 | 225 | 0.71105 | 0.28895 | Yes |
| 63.528 | 0.0000376477675 | 225 | 0.71105 | 0.28895 | Yes |
| 58.351 | 0.0000379996960 | 225 | 0.71105 | 0.28895 | Yes |
| 52.872 | 0.0000384054075 | 225 | 0.71105 | 0.28895 | Yes |
| 47.575 | 0.0000388424937 | 225 | 0.71105 | 0.28895 | Yes |
| 42.444 | 0.0000393112666 | 225 | 0.71105 | 0.28895 | Yes |
| 37.012 | 0.0000398708185 | 225 | 0.71105 | 0.28895 | Yes |
| 31.663 | 0.0000405022276 | 225 | 0.71105 | 0.28895 | Yes |
| 26.429 | 0.0000412354130 | 225 | 0.71105 | 0.28895 | Yes |
| 20.934 | 0.0000421798549 | 225 | 0.71105 | 0.28895 | Yes |
| 68.831 | 0.0000356239535 | 225 | 0.90921 | 0.09079 | Yes |
| 63.930 | 0.0000358140534 | 225 | 0.90921 | 0.09079 | Yes |
| 59.307 | 0.0000360074896 | 225 | 0.90921 | 0.09079 | Yes |
| 54.341 | 0.0000362253215 | 225 | 0.90921 | 0.09079 | Yes |
| 49.927 | 0.0000364351818 | 225 | 0.90921 | 0.09079 | Yes |
| 44.731 | 0.0000366945545 | 225 | 0.90921 | 0.09079 | Yes |
| 40.095 | 0.0000369398988 | 225 | 0.90921 | 0.09079 | Yes |
| 34.971 | 0.0000372328543 | 225 | 0.90921 | 0.09079 | Yes |
| 30.735 | 0.0000374925015 | 225 | 0.90921 | 0.09079 | Yes |
| 25.841 | 0.0000378143316 | 225 | 0.90921 | 0.09079 | Yes |
| 23.482 | 0.0000379852617 | 225 | 0.90921 | 0.09079 | Yes |
| 15.997 | 0.0000385757821 | 225 | 0.90921 | 0.09079 | Yes |
| 11.238 | 0.0000390076455 | 225 | 0.90921 | 0.09079 | Yes |
| 68.953 | 0.0000481904487 | 245 | 0.10560 | 0.89440 | Yes |
| 57.208 | 0.0000515596803 | 245 | 0.10560 | 0.89440 | Yes |
| 49.629 | 0.0000545702592 | 245 | 0.10560 | 0.89440 | Yes |
| 40.517 | 0.0000597550045 | 245 | 0.10560 | 0.89440 | Yes |
| 34.424 | 0.0000649603742 | 245 | 0.10560 | 0.89440 | Yes |
| 29.447 | 0.0000710934167 | 245 | 0.10560 | 0.89440 | Yes |
| 25.196 | 0.0000787277594 | 245 | 0.10560 | 0.89440 | Yes |
| 21.643 | 0.0000880591758 | 245 | 0.10560 | 0.89440 | Yes |
| 18.586 | 0.0000997804829 | 245 | 0.10560 | 0.89440 | Yes |
| 15.875 | 0.0001149689584 | 245 | 0.10560 | 0.89440 | Yes |
| 13.324 | 0.0001362212233 | 245 | 0.10560 | 0.89440 | Yes |
| 10.939 | 0.0001665556296 | 245 | 0.10560 | 0.89440 | Yes |
| 8.579 | 0.0002151925974 | 245 | 0.10560 | 0.89440 | Yes |
| 6.223 | 0.0003028467595 | 245 | 0.10560 | 0.89440 | Yes |
| 3.806 | 0.0005083884087 | 245 | 0.10560 | 0.89440 | Yes |
| 1.265 | 0.0015847860539 | 245 | 0.10560 | 0.89440 | Yes |
| 68.896 | 0.0000456975735 | 245 | 0.25147 | 0.74853 | Yes |
| 55.480 | 0.0000488376636 | 245 | 0.25147 | 0.74853 | Yes |
| 45.088 | 0.0000524851729 | 245 | 0.25147 | 0.74853 | Yes |
| 37.041 | 0.0000567633536 | 245 | 0.25147 | 0.74853 | Yes |
| 30.934 | 0.0000616979269 | 245 | 0.25147 | 0.74853 | Yes |
| 26.204 | 0.0000675128274 | 245 | 0.25147 | 0.74853 | Yes |
| 22.498 | 0.0000743936914 | 245 | 0.25147 | 0.74853 | Yes |
| 19.130 | 0.0000838785439 | 245 | 0.25147 | 0.74853 | Yes |
| 16.575 | 0.0000949126803 | 245 | 0.25147 | 0.74853 | Yes |
| 14.379 | 0.0001089087345 | 245 | 0.25147 | 0.74853 | Yes |
| 12.171 | 0.0001299714063 | 245 | 0.25147 | 0.74853 | Yes |
| 10.182 | 0.0001591596371 | 245 | 0.25147 | 0.74853 | Yes |

Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 8.167 | 0.0002058460272 | 245 | 0.25147 | 0.74853 | Yes |
| 6.059 | 0.0002907822041 | 245 | 0.25147 | 0.74853 | Yes |
| 3.737 | 0.0004987531172 | 245 | 0.25147 | 0.74853 | Yes |
| 1.182 | 0.0016835016835 | 245 | 0.25147 | 0.74853 | Yes |
| 69.031 | 0.0000417414534 | 245 | 0.50365 | 0.49635 | Yes |
| 64.442 | 0.0000423172951 | 245 | 0.50365 | 0.49635 | Yes |
| 59.470 | 0.0000430089028 | 245 | 0.50365 | 0.49635 | Yes |
| 54.654 | 0.0000437847541 | 245 | 0.50365 | 0.49635 | Yes |
| 49.798 | 0.0000446747677 | 245 | 0.50365 | 0.49635 | Yes |
| 44.823 | 0.0000457498399 | 245 | 0.50365 | 0.49635 | Yes |
| 40.137 | 0.0000469527655 | 245 | 0.50365 | 0.49635 | Yes |
| 35.095 | 0.0000485625486 | 245 | 0.50365 | 0.49635 | Yes |
| 30.213 | 0.0000505970451 | 245 | 0.50365 | 0.49635 | Yes |
| 25.376 | 0.0000534016875 | 245 | 0.50365 | 0.49635 | Yes |
| 20.573 | 0.0000577800890 | 245 | 0.50365 | 0.49635 | Yes |
| 69.042 | 0.0000390976268 | 245 | 0.71105 | 0.28895 | Yes |
| 64.182 | 0.0000394835551 | 245 | 0.71105 | 0.28895 | Yes |
| 58.841 | 0.0000399456739 | 245 | 0.71105 | 0.28895 | Yes |
| 54.941 | 0.0000403193291 | 245 | 0.71105 | 0.28895 | Yes |
| 49.385 | 0.0000409148562 | 245 | 0.71105 | 0.28895 | Yes |
| 44.239 | 0.0000415385893 | 245 | 0.71105 | 0.28895 | Yes |
| 39.256 | 0.0000422279465 | 245 | 0.71105 | 0.28895 | Yes |
| 34.043 | 0.0000430718870 | 245 | 0.71105 | 0.28895 | Yes |
| 29.624 | 0.0000439309406 | 245 | 0.71105 | 0.28895 | Yes |
| 24.157 | 0.0000452570601 | 245 | 0.71105 | 0.28895 | Yes |
| 18.997 | 0.0000469682025 | 245 | 0.71105 | 0.28895 | Yes |
| 68.926 | 0.0000371388249 | 245 | 0.90921 | 0.09079 | Yes |
| 63.374 | 0.0000374223486 | 245 | 0.90921 | 0.09079 | Yes |
| 57.687 | 0.0000377287304 | 245 | 0.90921 | 0.09079 | Yes |
| 52.013 | 0.0000380691335 | 245 | 0.90921 | 0.09079 | Yes |
| 46.110 | 0.0000384511862 | 245 | 0.90921 | 0.09079 | Yes |
| 40.397 | 0.0000388681592 | 245 | 0.90921 | 0.09079 | Yes |
| 34.971 | 0.0000392989075 | 245 | 0.90921 | 0.09079 | Yes |
| 29.357 | 0.0000398009950 | 245 | 0.90921 | 0.09079 | Yes |
| 23.315 | 0.0000404236397 | 245 | 0.90921 | 0.09079 | Yes |
| 17.497 | 0.0000411336432 | 245 | 0.90921 | 0.09079 | Yes |
| 11.846 | 0.0000419691946 | 245 | 0.90921 | 0.09079 | Yes |
| 68.418 | 0.0000429516365 | 255 | 0.50365 | 0.49635 | Yes |
| 63.922 | 0.0000435995814 | 255 | 0.50365 | 0.49635 | Yes |
| 59.345 | 0.0000443360674 | 255 | 0.50365 | 0.49635 | Yes |
| 55.723 | 0.0000449923513 | 255 | 0.50365 | 0.49635 | Yes |
| 50.245 | 0.0000461254613 | 255 | 0.50365 | 0.49635 | Yes |
| 45.746 | 0.0000472076665 | 255 | 0.50365 | 0.49635 | Yes |
| 41.210 | 0.0000485342652 | 255 | 0.50365 | 0.49635 | Yes |
| 36.441 | 0.0000502462064 | 255 | 0.50365 | 0.49635 | Yes |
| 32.023 | 0.0000522793810 | 255 | 0.50365 | 0.49635 | Yes |
| 27.634 | 0.0000550024751 | 255 | 0.50365 | 0.49635 | Yes |
| 22.818 | 0.0000594707107 | 255 | 0.50365 | 0.49635 | Yes |
| 18.165 | 0.0000671005838 | 255 | 0.50365 | 0.49635 | Yes |
| 68.980 | 0.0000508750509 | 265 | 0.10560 | 0.89440 | Yes |
| 59.626 | 0.0000539170755 | 265 | 0.10560 | 0.89440 | Yes |
| 51.662 | 0.0000574118728 | 265 | 0.10560 | 0.89440 | Yes |
| 45.014 | 0.0000613346418 | 265 | 0.10560 | 0.89440 | Yes |
| 39.419 | 0.0000657721652 | 265 | 0.10560 | 0.89440 | Yes |
| 34.460 | 0.0000710782572 | 265 | 0.10560 | 0.89440 | Yes |
| 30.257 | 0.0000771843161 | 265 | 0.10560 | 0.89440 | Yes |
| 26.580 | 0.0000844737287 | 265 | 0.10560 | 0.89440 | Yes |
| 23.281 | 0.0000933881210 | 265 | 0.10560 | 0.89440 | Yes |
| 20.372 | 0.0001041775185 | 265 | 0.10560 | 0.89440 | Yes |
| 17.697 | 0.0001178689298 | 265 | 0.10560 | 0.89440 | Yes |
| 15.189 | 0.0001359434475 | 265 | 0.10560 | 0.89440 | Yes |
| 12.832 | 0.0001602564103 | 265 | 0.10560 | 0.89440 | Yes |
| 10.538 | 0.0001953888238 | 265 | 0.10560 | 0.89440 | Yes |
| 8.288 | 0.0002502502503 | 265 | 0.10560 | 0.89440 | Yes |
| 6.015 | 0.0003487966516 | 265 | 0.10560 | 0.89440 | Yes |
| 3.740 | 0.0005701254276 | 265 | 0.10560 | 0.89440 | Yes |
| 1.408 | 0.001545950541 | 265 | 0.10560 | 0.89440 | Yes |
| 68.657 | 0.0000483675937 | 265 | 0.25147 | 0.74853 | Yes |
| 58.009 | 0.0000513109959 | 265 | 0.25147 | 0.74853 | Yes |
| 49.373 | 0.0000546179475 | 265 | 0.25147 | 0.74853 | Yes |
| 42.394 | 0.0000583260426 | 265 | 0.25147 | 0.74853 | Yes |
| 36.542 | 0.0000626841346 | 265 | 0.25147 | 0.74853 | Yes |
| 31.649 | 0.0000677874187 | 265 | 0.25147 | 0.74853 | Yes |
| 27.743 | 0.0000734969866 | 265 | 0.25147 | 0.74853 | Yes |
| 24.334 | 0.0000804569957 | 265 | 0.25147 | 0.74853 | Yes |
| 21.323 | 0.0000890551251 | 265 | 0.25147 | 0.74853 | Yes |
| 18.758 | 0.0000993048659 | 265 | 0.25147 | 0.74853 | Yes |
| 16.383 | 0.0001125999324 | 265 | 0.25147 | 0.74853 | Yes |
| 14.202 | 0.0001299545159 | 265 | 0.25147 | 0.74853 | Yes |
| 12.108 | 0.0001538698261 | 265 | 0.25147 | 0.74853 | Yes |
| 10.055 | 0.0001884303750 | 265 | 0.25147 | 0.74853 | Yes |
| 8.034 | 0.0002414875634 | 265 | 0.25147 | 0.74853 | Yes |
| 5.906 | 0.0003385240352 | 265 | 0.25147 | 0.74853 | Yes |
| 3.669 | 0.0005643340858 | 265 | 0.25147 | 0.74853 | Yes |
| 1.242 | 0.0017361111111 | 265 | 0.25147 | 0.74853 | Yes |
| 69.001 | 0.0000439966563 | 265 | 0.50365 | 0.49635 | Yes |
| 55.649 | 0.0000463994061 | 265 | 0.50365 | 0.49635 | Yes |
| 43.359 | 0.0000497240316 | 265 | 0.50365 | 0.49635 | Yes |
| 35.192 | 0.0000531603849 | 265 | 0.50365 | 0.49635 | Yes |
| 29.030 | 0.0000571265353 | 265 | 0.50365 | 0.49635 | Yes |
| 24.410 | 0.0000617627077 | 265 | 0.50365 | 0.49635 | Yes |
| 20.995 | 0.0000670555891 | 265 | 0.50365 | 0.49635 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 18.245 | 0.0000736105999 | 265 | 0.50365 | 0.49635 | Yes |
| 16.080 | 0.0000815328170 | 265 | 0.50365 | 0.49635 | Yes |
| 14.235 | 0.0000917010546 | 265 | 0.50365 | 0.49635 | Yes |
| 12.784 | 0.0001034447088 | 265 | 0.50365 | 0.49635 | Yes |
| 11.373 | 0.0001198897015 | 265 | 0.50365 | 0.49635 | Yes |
| 10.049 | 0.0001418842225 | 265 | 0.50365 | 0.49635 | Yes |
| 8.649 | 0.0001744896179 | 265 | 0.50365 | 0.49635 | Yes |
| 7.181 | 0.0002258355917 | 265 | 0.50365 | 0.49635 | Yes |
| 5.511 | 0.0003192848020 | 265 | 0.50365 | 0.49635 | Yes |
| 3.500 | 0.0005506607930 | 265 | 0.50365 | 0.49635 | Yes |
| 1.140 | 0.0018587360595 | 265 | 0.50365 | 0.49635 | Yes |
| 68.931 | 0.0000410441635 | 265 | 0.71105 | 0.28895 | Yes |
| 57.785 | 0.0000422725736 | 265 | 0.71105 | 0.28895 | Yes |
| 48.415 | 0.0000435938794 | 265 | 0.71105 | 0.28895 | Yes |
| 40.590 | 0.0000449984251 | 265 | 0.71105 | 0.28895 | Yes |
| 34.035 | 0.0000465354367 | 265 | 0.71105 | 0.28895 | Yes |
| 28.869 | 0.0000481185641 | 265 | 0.71105 | 0.28895 | Yes |
| 24.672 | 0.0000498206457 | 265 | 0.71105 | 0.28895 | Yes |
| 21.376 | 0.0000516129032 | 265 | 0.71105 | 0.28895 | Yes |
| 18.559 | 0.0000536682230 | 265 | 0.71105 | 0.28895 | Yes |
| 16.504 | 0.0000557506829 | 265 | 0.71105 | 0.28895 | Yes |
| 14.781 | 0.0000581598232 | 265 | 0.71105 | 0.28895 | Yes |
| 13.579 | 0.0000605070491 | 265 | 0.71105 | 0.28895 | Yes |
| 13.579 | 0.0000605070491 | 265 | 0.71105 | 0.28895 | Yes |
| 68.251 | 0.0000388440025 | 265 | 0.90921 | 0.09079 | Yes |
| 61.833 | 0.0000392680437 | 265 | 0.90921 | 0.09079 | Yes |
| 56.018 | 0.0000396998690 | 265 | 0.90921 | 0.09079 | Yes |
| 50.756 | 0.0000401300213 | 265 | 0.90921 | 0.09079 | Yes |
| 45.612 | 0.0000405959485 | 265 | 0.90921 | 0.09079 | Yes |
| 41.002 | 0.0000410509031 | 265 | 0.90921 | 0.09079 | Yes |
| 36.809 | 0.0000415092773 | 265 | 0.90921 | 0.09079 | Yes |
| 32.721 | 0.0000420150414 | 265 | 0.90921 | 0.09079 | Yes |
| 29.107 | 0.0000425115844 | 265 | 0.90921 | 0.09079 | Yes |
| 25.874 | 0.0000430107527 | 265 | 0.90921 | 0.09079 | Yes |
| 22.907 | 0.0000435198886 | 265 | 0.90921 | 0.09079 | Yes |
| 20.145 | 0.0000440606274 | 265 | 0.90921 | 0.09079 | Yes |
| 17.673 | 0.0000446030330 | 265 | 0.90921 | 0.09079 | Yes |
| 15.450 | 0.0000451528424 | 265 | 0.90921 | 0.09079 | Yes |
| 13.391 | 0.0000457414692 | 265 | 0.90921 | 0.09079 | Yes |
| 11.756 | 0.0000462727315 | 265 | 0.90921 | 0.09079 | Yes |
| 9.953 | 0.0000469461528 | 265 | 0.90921 | 0.09079 | Yes |
| 8.547 | 0.0000475511175 | 265 | 0.90921 | 0.09079 | Yes |
| 69.014 | 0.0000451691585 | 275 | 0.50365 | 0.49635 | Yes |
| 55.386 | 0.0000479363405 | 275 | 0.50365 | 0.49635 | Yes |
| 45.081 | 0.0000510334269 | 275 | 0.50365 | 0.49635 | Yes |
| 37.149 | 0.0000545791944 | 275 | 0.50365 | 0.49635 | Yes |
| 31.129 | 0.0000586372698 | 275 | 0.50365 | 0.49635 | Yes |
| 26.449 | 0.0000633793890 | 275 | 0.50365 | 0.49635 | Yes |
| 22.837 | 0.0000689369916 | 275 | 0.50365 | 0.49635 | Yes |
| 19.987 | 0.0000755229968 | 275 | 0.50365 | 0.49635 | Yes |
| 17.566 | 0.0000838855801 | 275 | 0.50365 | 0.49635 | Yes |
| 15.661 | 0.0000935278713 | 275 | 0.50365 | 0.49635 | Yes |
| 13.921 | 0.0001062022090 | 275 | 0.50365 | 0.49635 | Yes |
| 12.286 | 0.0001234872808 | 275 | 0.50365 | 0.49635 | Yes |
| 10.850 | 0.0001451589490 | 275 | 0.50365 | 0.49635 | Yes |
| 9.299 | 0.0001781895937 | 275 | 0.50365 | 0.49635 | Yes |
| 7.643 | 0.0002308402585 | 275 | 0.50365 | 0.49635 | Yes |
| 5.790 | 0.0003264773098 | 275 | 0.50365 | 0.49635 | Yes |
| 3.684 | 0.0005534034311 | 275 | 0.50365 | 0.49635 | Yes |
| 1.152 | 0.0019157088123 | 275 | 0.50365 | 0.49635 | Yes |
| 68.988 | 0.0000420751462 | 275 | 0.71105 | 0.28895 | Yes |
| 56.724 | 0.0000436338249 | 275 | 0.71105 | 0.28895 | Yes |
| 46.572 | 0.0000453576450 | 275 | 0.71105 | 0.28895 | Yes |
| 38.614 | 0.0000471809389 | 275 | 0.71105 | 0.28895 | Yes |
| 32.303 | 0.0000491424640 | 275 | 0.71105 | 0.28895 | Yes |
| 27.197 | 0.0000513267977 | 275 | 0.71105 | 0.28895 | Yes |
| 23.293 | 0.0000536682230 | 275 | 0.71105 | 0.28895 | Yes |
| 20.170 | 0.0000563126478 | 275 | 0.71105 | 0.28895 | Yes |
| 17.915 | 0.0000590179415 | 275 | 0.71105 | 0.28895 | Yes |
| 16.008 | 0.0000622703780 | 275 | 0.71105 | 0.28895 | Yes |
| 14.525 | 0.0000658978583 | 275 | 0.71105 | 0.28895 | Yes |
| 13.428 | 0.0000697058413 | 275 | 0.71105 | 0.28895 | Yes |
| 12.490 | 0.0000742115028 | 275 | 0.71105 | 0.28895 | Yes |
| 12.490 | 0.0000742115028 | 275 | 0.71105 | 0.28895 | Yes |
| 69.124 | 0.0000536020583 | 285 | 0.10560 | 0.89440 | Yes |
| 61.286 | 0.0000564812200 | 285 | 0.10560 | 0.89440 | Yes |
| 54.492 | 0.0000596801146 | 285 | 0.10560 | 0.89440 | Yes |
| 48.534 | 0.0000632671138 | 285 | 0.10560 | 0.89440 | Yes |
| 43.343 | 0.0000673038094 | 285 | 0.10560 | 0.89440 | Yes |
| 38.736 | 0.0000718597298 | 285 | 0.10560 | 0.89440 | Yes |
| 34.711 | 0.0000769882208 | 285 | 0.10560 | 0.89440 | Yes |
| 30.952 | 0.0000831462543 | 285 | 0.10560 | 0.89440 | Yes |
| 27.610 | 0.0000903260771 | 285 | 0.10560 | 0.89440 | Yes |
| 24.590 | 0.0000987751877 | 285 | 0.10560 | 0.89440 | Yes |
| 21.802 | 0.0001090393632 | 285 | 0.10560 | 0.89440 | Yes |
| 19.227 | 0.0001215509906 | 285 | 0.10560 | 0.89440 | Yes |
| 16.819 | 0.0001372495196 | 285 | 0.10560 | 0.89440 | Yes |
| 14.481 | 0.0001580777743 | 285 | 0.10560 | 0.89440 | Yes |
| 12.256 | 0.0001859427296 | 285 | 0.10560 | 0.89440 | Yes |
| 10.090 | 0.0002255808707 | 285 | 0.10560 | 0.89440 | Yes |
| 7.932 | 0.0002880184332 | 285 | 0.10560 | 0.89440 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 5.792 | 0.0003961965135 | 285 | 0.10560 | 0.89440 | Yes |
| 3.650 | 0.0006345177665 | 285 | 0.10560 | 0.89440 | Yes |
| 1.477 | 0.0015873015873 | 285 | 0.10560 | 0.89440 | Yes |
| 69.088 | 0.0000509580106 | 285 | 0.25147 | 0.74853 | Yes |
| 60.329 | 0.0000537056928 | 285 | 0.25147 | 0.74853 | Yes |
| 52.977 | 0.0000567472478 | 285 | 0.25147 | 0.74853 | Yes |
| 46.679 | 0.0000601503759 | 285 | 0.25147 | 0.74853 | Yes |
| 41.260 | 0.0000640286849 | 285 | 0.25147 | 0.74853 | Yes |
| 36.619 | 0.0000684041316 | 285 | 0.25147 | 0.74853 | Yes |
| 32.596 | 0.0000734052705 | 285 | 0.25147 | 0.74853 | Yes |
| 29.030 | 0.0000792958528 | 285 | 0.25147 | 0.74853 | Yes |
| 25.912 | 0.0000861029792 | 285 | 0.25147 | 0.74853 | Yes |
| 23.106 | 0.0000942418245 | 285 | 0.25147 | 0.74853 | Yes |
| 20.577 | 0.0001039609107 | 285 | 0.25147 | 0.74853 | Yes |
| 18.220 | 0.0001160766106 | 285 | 0.25147 | 0.74853 | Yes |
| 15.997 | 0.0001314924392 | 285 | 0.25147 | 0.74853 | Yes |
| 13.903 | 0.0001513546239 | 285 | 0.25147 | 0.74853 | Yes |
| 11.843 | 0.0001787629603 | 285 | 0.25147 | 0.74853 | Yes |
| 9.840 | 0.0002174858634 | 285 | 0.25147 | 0.74853 | Yes |
| 7.824 | 0.0002776235425 | 285 | 0.25147 | 0.74853 | Yes |
| 5.730 | 0.0003862495172 | 285 | 0.25147 | 0.74853 | Yes |
| 3.582 | 0.0006325110689 | 285 | 0.25147 | 0.74853 | Yes |
| 1.354 | 0.0017123287671 | 285 | 0.25147 | 0.74853 | Yes |
| 69.189 | 0.0000463800380 | 285 | 0.50365 | 0.49635 | Yes |
| 57.633 | 0.0000488997555 | 285 | 0.50365 | 0.49635 | Yes |
| 48.491 | 0.0000516982888 | 285 | 0.50365 | 0.49635 | Yes |
| 41.194 | 0.0000548305735 | 285 | 0.50365 | 0.49635 | Yes |
| 35.359 | 0.0000583532707 | 285 | 0.50365 | 0.49635 | Yes |
| 30.659 | 0.0000623908161 | 285 | 0.50365 | 0.49635 | Yes |
| 26.842 | 0.0000670376081 | 285 | 0.50365 | 0.49635 | Yes |
| 23.732 | 0.0000723903287 | 285 | 0.50365 | 0.49635 | Yes |
| 21.142 | 0.0000787091696 | 285 | 0.50365 | 0.49635 | Yes |
| 18.932 | 0.0000862143288 | 285 | 0.50365 | 0.49635 | Yes |
| 16.990 | 0.0000954289531 | 285 | 0.50365 | 0.49635 | Yes |
| 15.270 | 0.0001066666667 | 285 | 0.50365 | 0.49635 | Yes |
| 13.678 | 0.0001208751360 | 285 | 0.50365 | 0.49635 | Yes |
| 12.150 | 0.0001394116827 | 285 | 0.50365 | 0.49635 | Yes |
| 10.616 | 0.0001651527663 | 285 | 0.50365 | 0.49635 | Yes |
| 9.050 | 0.0002021018593 | 285 | 0.50365 | 0.49635 | Yes |
| 7.376 | 0.0002606202763 | 285 | 0.50365 | 0.49635 | Yes |
| 5.543 | 0.0003660322108 | 285 | 0.50365 | 0.49635 | Yes |
| 3.502 | 0.0006146281500 | 285 | 0.50365 | 0.49635 | Yes |
| 1.192 | 0.0019157088123 | 285 | 0.50365 | 0.49635 | Yes |
| 69.080 | 0.0000431276146 | 285 | 0.71105 | 0.28895 | Yes |
| 55.607 | 0.0000451019304 | 285 | 0.71105 | 0.28895 | Yes |
| 44.919 | 0.0000473014522 | 285 | 0.71105 | 0.28895 | Yes |
| 35.358 | 0.0000502008032 | 285 | 0.71105 | 0.28895 | Yes |
| 26.656 | 0.0000546060176 | 285 | 0.71105 | 0.28895 | Yes |
| 21.011 | 0.0000598479861 | 285 | 0.71105 | 0.28895 | Yes |
| 17.501 | 0.0000658197854 | 285 | 0.71105 | 0.28895 | Yes |
| 15.302 | 0.0000722804481 | 285 | 0.71105 | 0.28895 | Yes |
| 13.685 | 0.0000799808046 | 285 | 0.71105 | 0.28895 | Yes |
| 12.389 | 0.0000897263347 | 285 | 0.71105 | 0.28895 | Yes |
| 11.337 | 0.0001015640869 | 285 | 0.71105 | 0.28895 | Yes |
| 10.346 | 0.0001179662616 | 285 | 0.71105 | 0.28895 | Yes |
| 9.405 | 0.0001399188471 | 285 | 0.71105 | 0.28895 | Yes |
| 8.387 | 0.0001721170396 | 285 | 0.71105 | 0.28895 | Yes |
| 7.189 | 0.000226675573 | 285 | 0.71105 | 0.28895 | Yes |
| 5.658 | 0.0003166561115 | 285 | 0.71105 | 0.28895 | Yes |
| 3.656 | 0.0005515719801 | 285 | 0.71105 | 0.28895 | Yes |
| 1.088 | 0.0020833333333 | 285 | 0.71105 | 0.28895 | Yes |
| 69.019 | 0.0000406140850 | 285 | 0.90921 | 0.09079 | Yes |
| 57.355 | 0.0000416597234 | 285 | 0.90921 | 0.09079 | Yes |
| 47.721 | 0.0000427386956 | 285 | 0.90921 | 0.09079 | Yes |
| 39.762 | 0.0000438461876 | 285 | 0.90921 | 0.09079 | Yes |
| 32.843 | 0.0000450511330 | 285 | 0.90921 | 0.09079 | Yes |
| 27.142 | 0.0000463177397 | 285 | 0.90921 | 0.09079 | Yes |
| 22.447 | 0.0000476621705 | 285 | 0.90921 | 0.09079 | Yes |
| 18.648 | 0.0000490966222 | 285 | 0.90921 | 0.09079 | Yes |
| 15.654 | 0.0000505996053 | 285 | 0.90921 | 0.09079 | Yes |
| 13.219 | 0.0000522356874 | 285 | 0.90921 | 0.09079 | Yes |
| 11.374 | 0.0000539723661 | 285 | 0.90921 | 0.09079 | Yes |
| 10.034 | 0.0000557444674 | 285 | 0.90921 | 0.09079 | Yes |
| 9.013 | 0.0000576568266 | 285 | 0.90921 | 0.09079 | Yes |
| 69.055 | 0.0000557537913 | 300 | 0.10560 | 0.89440 | Yes |
| 61.675 | 0.0000587130108 | 300 | 0.10560 | 0.89440 | Yes |
| 55.165 | 0.0000620424370 | 300 | 0.10560 | 0.89440 | Yes |
| 49.506 | 0.0000657073395 | 300 | 0.10560 | 0.89440 | Yes |
| 44.370 | 0.0000699007409 | 300 | 0.10560 | 0.89440 | Yes |
| 39.817 | 0.0000746491490 | 300 | 0.10560 | 0.89440 | Yes |
| 35.681 | 0.0000801538955 | 300 | 0.10560 | 0.89440 | Yes |
| 31.967 | 0.0000864453665 | 300 | 0.10560 | 0.89440 | Yes |
| 28.534 | 0.0000940026321 | 300 | 0.10560 | 0.89440 | Yes |
| 25.493 | 0.0001026377912 | 300 | 0.10560 | 0.89440 | Yes |
| 22.642 | 0.0001131221719 | 300 | 0.10560 | 0.89440 | Yes |
| 19.933 | 0.0001262785705 | 300 | 0.10560 | 0.89440 | Yes |
| 17.400 | 0.0001427144284 | 300 | 0.10560 | 0.89440 | Yes |
| 14.971 | 0.0001642575558 | 300 | 0.10560 | 0.89440 | Yes |
| 12.682 | 0.0001927525058 | 300 | 0.10560 | 0.89440 | Yes |
| 10.413 | 0.0002340823970 | 300 | 0.10560 | 0.89440 | Yes |
| 8.196 | 0.0002973535534 | 300 | 0.10560 | 0.89440 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 5.999 | 0.0004071661238 | 300 | 0.10560 | 0.89440 | Yes |
| 3.767 | 0.0006518904824 | 300 | 0.10560 | 0.89440 | Yes |
| 1.537 | 0.0016129032258 | 300 | 0.10560 | 0.89440 | Yes |
| 69.107 | 0.0000533646406 | 300 | 0.25147 | 0.74853 | Yes |
| 60.931 | 0.0000562619557 | 300 | 0.25147 | 0.74853 | Yes |
| 54.037 | 0.0000594247682 | 300 | 0.25147 | 0.74853 | Yes |
| 48.072 | 0.0000629485081 | 300 | 0.25147 | 0.74853 | Yes |
| 42.827 | 0.0000669792364 | 300 | 0.25147 | 0.74853 | Yes |
| 38.228 | 0.0000715409930 | 300 | 0.25147 | 0.74853 | Yes |
| 34.097 | 0.0000768875903 | 300 | 0.25147 | 0.74853 | Yes |
| 30.514 | 0.0000829600133 | 300 | 0.25147 | 0.74853 | Yes |
| 27.295 | 0.0000900576369 | 300 | 0.25147 | 0.74853 | Yes |
| 24.350 | 0.0000985998817 | 300 | 0.25147 | 0.74853 | Yes |
| 21.667 | 0.0001088257699 | 300 | 0.25147 | 0.74853 | Yes |
| 19.169 | 0.0001214771623 | 300 | 0.25147 | 0.74853 | Yes |
| 16.816 | 0.0001374381528 | 300 | 0.25147 | 0.74853 | Yes |
| 14.565 | 0.0001582528881 | 300 | 0.25147 | 0.74853 | Yes |
| 12.396 | 0.0001862891207 | 300 | 0.25147 | 0.74853 | Yes |
| 10.244 | 0.0002268602541 | 300 | 0.25147 | 0.74853 | Yes |
| 8.099 | 0.0002900232019 | 300 | 0.25147 | 0.74853 | Yes |
| 5.937 | 0.0004006410256 | 300 | 0.25147 | 0.74853 | Yes |
| 3.713 | 0.0006523157208 | 300 | 0.25147 | 0.74853 | Yes |
| 1.436 | 0.0017211703959 | 300 | 0.25147 | 0.74853 | Yes |
| 69.028 | 0.0000483863163 | 300 | 0.50365 | 0.49635 | Yes |
| 58.681 | 0.0000510021931 | 300 | 0.50365 | 0.49635 | Yes |
| 50.230 | 0.0000539345235 | 300 | 0.50365 | 0.49635 | Yes |
| 43.426 | 0.0000571820677 | 300 | 0.50365 | 0.49635 | Yes |
| 37.763 | 0.0000608828006 | 300 | 0.50365 | 0.49635 | Yes |
| 33.118 | 0.0000650702759 | 300 | 0.50365 | 0.49635 | Yes |
| 29.248 | 0.0000699202909 | 300 | 0.50365 | 0.49635 | Yes |
| 26.056 | 0.0000754204691 | 300 | 0.50365 | 0.49635 | Yes |
| 23.267 | 0.0000820008200 | 300 | 0.50365 | 0.49635 | Yes |
| 20.829 | 0.0000899038029 | 300 | 0.50365 | 0.49635 | Yes |
| 18.707 | 0.0000993147284 | 300 | 0.50365 | 0.49635 | Yes |
| 16.744 | 0.0001110247585 | 300 | 0.50365 | 0.49635 | Yes |
| 14.914 | 0.0001259128683 | 300 | 0.50365 | 0.49635 | Yes |
| 13.165 | 0.0001451800232 | 300 | 0.50365 | 0.49635 | Yes |
| 11.413 | 0.0001718803713 | 300 | 0.50365 | 0.49635 | Yes |
| 9.643 | 0.0002101723413 | 300 | 0.50365 | 0.49635 | Yes |
| 7.789 | 0.0002706359946 | 300 | 0.50365 | 0.49635 | Yes |
| 5.819 | 0.0003780718336 | 300 | 0.50365 | 0.49635 | Yes |
| 3.652 | 0.0006333122229 | 300 | 0.50365 | 0.49635 | Yes |
| 1.262 | 0.0019379844961 | 300 | 0.50365 | 0.49635 | Yes |
| 69.024 | 0.0000448651801 | 300 | 0.71105 | 0.28895 | Yes |
| 55.166 | 0.0000473036897 | 300 | 0.71105 | 0.28895 | Yes |
| 44.719 | 0.0000500175061 | 300 | 0.71105 | 0.28895 | Yes |
| 36.720 | 0.0000530701056 | 300 | 0.71105 | 0.28895 | Yes |
| 30.675 | 0.0000565418975 | 300 | 0.71105 | 0.28895 | Yes |
| 26.095 | 0.0000604741171 | 300 | 0.71105 | 0.28895 | Yes |
| 22.632 | 0.0000649814803 | 300 | 0.71105 | 0.28895 | Yes |
| 19.974 | 0.0000701360640 | 300 | 0.71105 | 0.28895 | Yes |
| 17.845 | 0.0000763883584 | 300 | 0.71105 | 0.28895 | Yes |
| 16.111 | 0.0000838855801 | 300 | 0.71105 | 0.28895 | Yes |
| 14.704 | 0.0000927213723 | 300 | 0.71105 | 0.28895 | Yes |
| 13.465 | 0.0001034661148 | 300 | 0.71105 | 0.28895 | Yes |
| 12.271 | 0.0001177163037 | 300 | 0.71105 | 0.28895 | Yes |
| 11.181 | 0.0001354646437 | 300 | 0.71105 | 0.28895 | Yes |
| 9.989 | 0.0001611084260 | 300 | 0.71105 | 0.28895 | Yes |
| 8.735 | 0.0001972775695 | 300 | 0.71105 | 0.28895 | Yes |
| 7.292 | 0.0002551020408 | 300 | 0.71105 | 0.28895 | Yes |
| 5.602 | 0.0003602305476 | 300 | 0.71105 | 0.28895 | Yes |
| 3.567 | 0.0006172839506 | 300 | 0.71105 | 0.28895 | Yes |
| 1.147 | 0.0021052631579 | 300 | 0.71105 | 0.28895 | Yes |
| 69.020 | 0.0000420486082 | 300 | 0.90921 | 0.09079 | Yes |
| 55.550 | 0.0000435521101 | 300 | 0.90921 | 0.09079 | Yes |
| 43.810 | 0.0000453370812 | 300 | 0.90921 | 0.09079 | Yes |
| 34.664 | 0.0000472656804 | 300 | 0.90921 | 0.09079 | Yes |
| 26.591 | 0.0000497784857 | 300 | 0.90921 | 0.09079 | Yes |
| 19.704 | 0.0000533049041 | 300 | 0.90921 | 0.09079 | Yes |
| 14.523 | 0.0000586235198 | 300 | 0.90921 | 0.09079 | Yes |
| 11.758 | 0.0000652869361 | 300 | 0.90921 | 0.09079 | Yes |
| 10.406 | 0.0000732118017 | 300 | 0.90921 | 0.09079 | Yes |
| 9.571 | 0.0000844880027 | 300 | 0.90921 | 0.09079 | Yes |
| 9.037 | 0.0000984736583 | 300 | 0.90921 | 0.09079 | Yes |
| 8.608 | 0.0001160900859 | 300 | 0.90921 | 0.09079 | Yes |
| 8.212 | 0.0001374381528 | 300 | 0.90921 | 0.09079 | Yes |
| 7.677 | 0.0001683501684 | 300 | 0.90921 | 0.09079 | Yes |
| 6.831 | 0.0002203613927 | 300 | 0.90921 | 0.09079 | Yes |
| 5.587 | 0.0003135779241 | 300 | 0.90921 | 0.09079 | Yes |
| 3.708 | 0.0005509641873 | 300 | 0.90921 | 0.09079 | Yes |
| 1.031 | 0.0023094688222 | 300 | 0.90921 | 0.09079 | Yes |
| 34.747 | 0.0000878657411 | 320 | 0.10560 | 0.89440 | Yes |
| 30.700 | 0.0000961076406 | 320 | 0.10560 | 0.89440 | Yes |
| 27.037 | 0.0001060670344 | 320 | 0.10560 | 0.89440 | Yes |
| 23.668 | 0.0001183291918 | 320 | 0.10560 | 0.89440 | Yes |
| 20.550 | 0.0001336183859 | 320 | 0.10560 | 0.89440 | Yes |
| 17.649 | 0.0001533272002 | 320 | 0.10560 | 0.89440 | Yes |
| 14.819 | 0.0001804402743 | 320 | 0.10560 | 0.89440 | Yes |
| 12.114 | 0.0002189621196 | 320 | 0.10560 | 0.89440 | Yes |
| 9.397 | 0.0002810567735 | 320 | 0.10560 | 0.89440 | Yes |
| 6.805 | 0.0003875968992 | 320 | 0.10560 | 0.89440 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 4.181 | 0.0006317119394 | 320 | 0.10560 | 0.89440 | Yes |
| 1.740 | 0.0015197568389 | 320 | 0.10560 | 0.89440 | Yes |
| 69.011 | 0.0000559002739 | 320 | 0.25147 | 0.74853 | Yes |
| 61.506 | 0.0000588754784 | 320 | 0.25147 | 0.74853 | Yes |
| 54.928 | 0.0000622432466 | 320 | 0.25147 | 0.74853 | Yes |
| 50.951 | 0.0000647081662 | 320 | 0.25147 | 0.74853 | Yes |
| 45.125 | 0.0000692376930 | 320 | 0.25147 | 0.74853 | Yes |
| 39.687 | 0.0000748727164 | 320 | 0.25147 | 0.74853 | Yes |
| 35.619 | 0.0000804052424 | 320 | 0.25147 | 0.74853 | Yes |
| 32.020 | 0.0000865875833 | 320 | 0.25147 | 0.74853 | Yes |
| 28.675 | 0.0000940733772 | 320 | 0.25147 | 0.74853 | Yes |
| 25.733 | 0.0001025956705 | 320 | 0.25147 | 0.74853 | Yes |
| 22.962 | 0.0001129943503 | 320 | 0.25147 | 0.74853 | Yes |
| 20.261 | 0.0001263743207 | 320 | 0.25147 | 0.74853 | Yes |
| 17.748 | 0.0001428979708 | 320 | 0.25147 | 0.74853 | Yes |
| 15.405 | 0.0001638538424 | 320 | 0.25147 | 0.74853 | Yes |
| 13.081 | 0.0001926411096 | 320 | 0.25147 | 0.74853 | Yes |
| 10.804 | 0.0002339181287 | 320 | 0.25147 | 0.74853 | Yes |
| 8.566 | 0.0002965599051 | 320 | 0.25147 | 0.74853 | Yes |
| 6.308 | 0.0004061738424 | 320 | 0.25147 | 0.74853 | Yes |
| 3.923 | 0.0006605019815 | 320 | 0.25147 | 0.74853 | Yes |
| 1.554 | 0.0016977928693 | 320 | 0.25147 | 0.74853 | Yes |
| 69.044 | 0.0000510334269 | 320 | 0.50365 | 0.49635 | Yes |
| 59.508 | 0.0000538502962 | 320 | 0.50365 | 0.49635 | Yes |
| 51.900 | 0.0000569281567 | 320 | 0.50365 | 0.49635 | Yes |
| 45.580 | 0.0000603463883 | 320 | 0.50365 | 0.49635 | Yes |
| 40.180 | 0.0000642590927 | 320 | 0.50365 | 0.49635 | Yes |
| 35.685 | 0.0000686436024 | 320 | 0.50365 | 0.49635 | Yes |
| 31.758 | 0.0000737463127 | 320 | 0.50365 | 0.49635 | Yes |
| 28.435 | 0.0000795861520 | 320 | 0.50365 | 0.49635 | Yes |
| 25.458 | 0.0000865875833 | 320 | 0.50365 | 0.49635 | Yes |
| 22.859 | 0.0000947777462 | 320 | 0.50365 | 0.49635 | Yes |
| 20.472 | 0.0001047449461 | 320 | 0.50365 | 0.49635 | Yes |
| 18.276 | 0.0001172058134 | 320 | 0.50365 | 0.49635 | Yes |
| 16.233 | 0.0001325205407 | 320 | 0.50365 | 0.49635 | Yes |
| 14.233 | 0.0001528584531 | 320 | 0.50365 | 0.49635 | Yes |
| 12.261 | 0.0001806032147 | 320 | 0.50365 | 0.49635 | Yes |
| 10.290 | 0.0002205071665 | 320 | 0.50365 | 0.49635 | Yes |
| 8.230 | 0.0002836879433 | 320 | 0.50365 | 0.49635 | Yes |
| 6.074 | 0.0003971405878 | 320 | 0.50365 | 0.49635 | Yes |
| 3.800 | 0.0006587615283 | 320 | 0.50365 | 0.49635 | Yes |
| 1.353 | 0.0019305019305 | 320 | 0.50365 | 0.49635 | Yes |
| 68.951 | 0.0000472902677 | 320 | 0.71105 | 0.28895 | Yes |
| 56.959 | 0.0000498902415 | 320 | 0.71105 | 0.28895 | Yes |
| 47.500 | 0.0000528345749 | 320 | 0.71105 | 0.28895 | Yes |
| 40.063 | 0.0000561671534 | 320 | 0.71105 | 0.28895 | Yes |
| 34.288 | 0.0000598945855 | 320 | 0.71105 | 0.28895 | Yes |
| 29.742 | 0.0000641972138 | 320 | 0.71105 | 0.28895 | Yes |
| 26.138 | 0.0000691323885 | 320 | 0.71105 | 0.28895 | Yes |
| 23.221 | 0.0000748727164 | 320 | 0.71105 | 0.28895 | Yes |
| 20.797 | 0.0000816459830 | 320 | 0.71105 | 0.28895 | Yes |
| 18.747 | 0.0000898311175 | 320 | 0.71105 | 0.28895 | Yes |
| 16.988 | 0.0000997506234 | 320 | 0.71105 | 0.28895 | Yes |
| 15.338 | 0.0001122838536 | 320 | 0.71105 | 0.28895 | Yes |
| 13.797 | 0.0001283532281 | 320 | 0.71105 | 0.28895 | Yes |
| 12.287 | 0.0001496110114 | 320 | 0.71105 | 0.28895 | Yes |
| 10.719 | 0.0001796299623 | 320 | 0.71105 | 0.28895 | Yes |
| 9.068 | 0.0002242152466 | 320 | 0.71105 | 0.28895 | Yes |
| 7.231 | 0.0002991325157 | 320 | 0.71105 | 0.28895 | Yes |
| 5.144 | 0.0004488330341 | 320 | 0.71105 | 0.28895 | Yes |
| 2.761 | 0.0008984725966 | 320 | 0.71105 | 0.28895 | Yes |
| 1.224 | 0.0021186440678 | 320 | 0.71105 | 0.28895 | Yes |
| 69.065 | 0.0000441423148 | 320 | 0.90921 | 0.09079 | Yes |
| 55.533 | 0.0000460935699 | 320 | 0.90921 | 0.09079 | Yes |
| 41.924 | 0.0000490148025 | 320 | 0.90921 | 0.09079 | Yes |
| 31.439 | 0.0000527398344 | 320 | 0.90921 | 0.09079 | Yes |
| 24.524 | 0.0000570353049 | 320 | 0.90921 | 0.09079 | Yes |
| 19.987 | 0.0000620770998 | 320 | 0.90921 | 0.09079 | Yes |
| 17.288 | 0.0000673763644 | 320 | 0.90921 | 0.09079 | Yes |
| 15.306 | 0.0000741125028 | 320 | 0.90921 | 0.09079 | Yes |
| 13.907 | 0.0000821287779 | 320 | 0.90921 | 0.09079 | Yes |
| 12.841 | 0.0000918779860 | 320 | 0.90921 | 0.09079 | Yes |
| 11.919 | 0.0001044277360 | 320 | 0.90921 | 0.09079 | Yes |
| 11.058 | 0.0001208605270 | 320 | 0.90921 | 0.09079 | Yes |
| 10.159 | 0.0001433691756 | 320 | 0.90921 | 0.09079 | Yes |
| 9.113 | 0.0001764602082 | 320 | 0.90921 | 0.09079 | Yes |
| 7.881 | 0.0002263980077 | 320 | 0.90921 | 0.09079 | Yes |
| 6.126 | 0.0003286230693 | 320 | 0.90921 | 0.09079 | Yes |
| 3.955 | 0.0005727376861 | 320 | 0.90921 | 0.09079 | Yes |
| 1.111 | 0.0022988505747 | 320 | 0.90921 | 0.09079 | Yes |
| 69.189 | 0.0000627667587 | 350 | 0.10560 | 0.89440 | Yes |
| 62.799 | 0.0000660938533 | 350 | 0.10560 | 0.89440 | Yes |
| 57.018 | 0.0000697982830 | 350 | 0.10560 | 0.89440 | Yes |
| 51.735 | 0.0000739644970 | 350 | 0.10560 | 0.89440 | Yes |
| 46.821 | 0.0000787401575 | 350 | 0.10560 | 0.89440 | Yes |
| 42.587 | 0.0000838433806 | 350 | 0.10560 | 0.89440 | Yes |
| 38.449 | 0.0000899928006 | 350 | 0.10560 | 0.89440 | Yes |
| 34.625 | 0.0000971062342 | 350 | 0.10560 | 0.89440 | Yes |
| 31.132 | 0.0001052742394 | 350 | 0.10560 | 0.89440 | Yes |
| 27.855 | 0.0001150350857 | 350 | 0.10560 | 0.89440 | Yes |
| 24.756 | 0.0001268391679 | 350 | 0.10560 | 0.89440 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------------|-------------------|------------------|--------------------|
| 21.856 | 0.0001412229911 | 350 | 0.10560 | 0.89440 | Yes |
| 19.062 | 0.0001594642003 | 350 | 0.10560 | 0.89440 | Yes |
| 16.417 | 0.0001827819411 | 350 | 0.10560 | 0.89440 | Yes |
| 13.867 | 0.0002141327623 | 350 | 0.10560 | 0.89440 | Yes |
| 11.366 | 0.0002592688618 | 350 | 0.10560 | 0.89440 | Yes |
| 8.925 | 0.0003281916639 | 350 | 0.10560 | 0.89440 | Yes |
| 6.550 | 0.0004452359751 | 350 | 0.10560 | 0.89440 | Yes |
| 4.182 | 0.0006949270327 | 350 | 0.10560 | 0.89440 | Yes |
| 1.840 | 0.0015748031496 | 350 | 0.10560 | 0.89440 | Yes |
| 69.195 | 0.0000600925425 | 350 | 0.25147 | 0.74853 | Yes |
| 62.429 | 0.0000632871337 | 350 | 0.25147 | 0.74853 | Yes |
| 56.348 | 0.0000668538575 | 350 | 0.25147 | 0.74853 | Yes |
| 50.943 | 0.0000708315625 | 350 | 0.25147 | 0.74853 | Yes |
| 46.046 | 0.0000753579503 | 350 | 0.25147 | 0.74853 | Yes |
| 41.551 | 0.0000805542130 | 350 | 0.25147 | 0.74853 | Yes |
| 37.578 | 0.0000862887221 | 350 | 0.25147 | 0.74853 | Yes |
| 33.822 | 0.0000931532371 | 350 | 0.25147 | 0.74853 | Yes |
| 30.428 | 0.0001010611420 | 350 | 0.25147 | 0.74853 | Yes |
| 27.254 | 0.0001105094486 | 350 | 0.25147 | 0.74853 | Yes |
| 24.223 | 0.0001221150324 | 350 | 0.25147 | 0.74853 | Yes |
| 21.446 | 0.0001359804188 | 350 | 0.25147 | 0.74853 | Yes |
| 18.790 | 0.0001535390757 | 350 | 0.25147 | 0.74853 | Yes |
| 16.208 | 0.0001766472355 | 350 | 0.25147 | 0.74853 | Yes |
| 13.711 | 0.0002077274616 | 350 | 0.25147 | 0.74853 | Yes |
| 8.875 | 0.0003206155819 | 350 | 0.25147 | 0.74853 | Yes |
| 6.486 | 0.0004395604396 | 350 | 0.25147 | 0.74853 | Yes |
| 4.097 | 0.0006993006993 | 350 | 0.25147 | 0.74853 | Yes |
| 1.687 | 0.0017064846416 | 350 | 0.25147 | 0.74853 | Yes |
| 69.156 | 0.0000551571980 | 350 | 0.50365 | 0.49635 | Yes |
| 61.236 | 0.0000581057525 | 350 | 0.50365 | 0.49635 | Yes |
| 54.438 | 0.0000613986615 | 350 | 0.50365 | 0.49635 | Yes |
| 48.458 | 0.0000651805501 | 350 | 0.50365 | 0.49635 | Yes |
| 43.405 | 0.0000693000693 | 350 | 0.50365 | 0.49635 | Yes |
| 38.917 | 0.0000740795614 | 350 | 0.50365 | 0.49635 | Yes |
| 34.980 | 0.0000794975753 | 350 | 0.50365 | 0.49635 | Yes |
| 31.453 | 0.0000858369099 | 350 | 0.50365 | 0.49635 | Yes |
| 28.285 | 0.0000932835821 | 350 | 0.50365 | 0.49635 | Yes |
| 25.426 | 0.0001020304051 | 350 | 0.50365 | 0.49635 | Yes |
| 22.752 | 0.0001127268628 | 350 | 0.50365 | 0.49635 | Yes |
| 20.228 | 0.0001261034048 | 350 | 0.50365 | 0.49635 | Yes |
| 17.857 | 0.0001427551749 | 350 | 0.50365 | 0.49635 | Yes |
| 15.571 | 0.0001643925695 | 350 | 0.50365 | 0.49635 | Yes |
| 13.325 | 0.0001939111887 | 350 | 0.50365 | 0.49635 | Yes |
| 11.077 | 0.0002364625207 | 350 | 0.50365 | 0.49635 | Yes |
| 8.801 | 0.0003029385035 | 350 | 0.50365 | 0.49635 | Yes |
| 6.454 | 0.0004219409283 | 350 | 0.50365 | 0.49635 | Yes |
| 4.034 | 0.0006915629322 | 350 | 0.50365 | 0.49635 | Yes |
| 1.476 | 0.0019531250000 | 350 | 0.50365 | 0.49635 | Yes |
| 69.088 | 0.0000511325868 | 350 | 0.71105 | 0.28895 | Yes |
| 59.363 | 0.0000539199827 | 350 | 0.71105 | 0.28895 | Yes |
| 51.469 | 0.0000569930468 | 350 | 0.71105 | 0.28895 | Yes |
| 45.039 | 0.0000603937674 | 350 | 0.71105 | 0.28895 | Yes |
| 39.580 | 0.0000643459237 | 350 | 0.71105 | 0.28895 | Yes |
| 35.089 | 0.0000687757909 | 350 | 0.71105 | 0.28895 | Yes |
| 31.309 | 0.0000738552437 | 350 | 0.71105 | 0.28895 | Yes |
| 28.076 | 0.0000797575371 | 350 | 0.71105 | 0.28895 | Yes |
| 25.267 | 0.0000867302689 | 350 | 0.71105 | 0.28895 | Yes |
| 22.802 | 0.0000949667616 | 350 | 0.71105 | 0.28895 | Yes |
| 20.562 | 0.0001049979000 | 350 | 0.71105 | 0.28895 | Yes |
| 18.453 | 0.0001176885960 | 350 | 0.71105 | 0.28895 | Yes |
| 16.502 | 0.0001333333333 | 350 | 0.71105 | 0.28895 | Yes |
| 14.597 | 0.0001537042730 | 350 | 0.71105 | 0.28895 | Yes |
| 12.664 | 0.0001818843216 | 350 | 0.71105 | 0.28895 | Yes |
| 10.712 | 0.0002221728505 | 350 | 0.71105 | 0.28895 | Yes |
| 8.374 | 0.0002968239834 | 350 | 0.71105 | 0.28895 | Yes |
| 6.421 | 0.0004016064257 | 350 | 0.71105 | 0.28895 | Yes |
| 3.980 | 0.0006784260516 | 350 | 0.71105 | 0.28895 | Yes |
| 1.333 | 0.0021321961620 | 350 | 0.71105 | 0.28895 | Yes |
| 69.093 | 0.0000476122459 | 350 | 0.90921 | 0.09079 | Yes |
| 56.576 | 0.0000501806503 | 350 | 0.90921 | 0.09079 | Yes |
| 46.868 | 0.0000530532124 | 350 | 0.90921 | 0.09079 | Yes |
| 39.302 | 0.0000563253351 | 350 | 0.90921 | 0.09079 | Yes |
| 33.571 | 0.0000599628230 | 350 | 0.90921 | 0.09079 | Yes |
| 29.105 | 0.0000641395677 | 350 | 0.90921 | 0.09079 | Yes |
| 25.639 | 0.0000689179876 | 350 | 0.90921 | 0.09079 | Yes |
| 22.896 | 0.0000745267551 | 350 | 0.90921 | 0.09079 | Yes |
| 20.684 | 0.0000810635538 | 350 | 0.90921 | 0.09079 | Yes |
| 18.865 | 0.0000887705282 | 350 | 0.90921 | 0.09079 | Yes |
| 17.249 | 0.0000982607841 | 350 | 0.90921 | 0.09079 | Yes |
| 15.798 | 0.0001099263493 | 350 | 0.90921 | 0.09079 | Yes |
| 14.396 | 0.0001249531426 | 350 | 0.90921 | 0.09079 | Yes |
| 13.019 | 0.0001446340758 | 350 | 0.90921 | 0.09079 | Yes |
| 11.601 | 0.0001709693965 | 350 | 0.90921 | 0.09079 | Yes |
| 10.053 | 0.0002095118374 | 350 | 0.90921 | 0.09079 | Yes |
| 8.306 | 0.0002711496746 | 350 | 0.90921 | 0.09079 | Yes |
| 6.290 | 0.0003849114704 | 350 | 0.90921 | 0.09079 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 3.957 | 0.0006591957811 | 350 | 0.90921 | 0.09079 | Yes |
| 1.220 | 0.0023041474654 | 350 | 0.90921 | 0.09079 | Yes |
| 68.655 | 0.0000701557458 | 400 | 0.10560 | 0.89440 | Yes |
| 63.076 | 0.0000737517516 | 400 | 0.10560 | 0.89440 | Yes |
| 57.528 | 0.0000780822987 | 400 | 0.10560 | 0.89440 | Yes |
| 51.633 | 0.0000837591088 | 400 | 0.10560 | 0.89440 | Yes |
| 45.922 | 0.0000907605736 | 400 | 0.10560 | 0.89440 | Yes |
| 40.264 | 0.0000997506234 | 400 | 0.10560 | 0.89440 | Yes |
| 34.122 | 0.0001131605749 | 400 | 0.10560 | 0.89440 | Yes |
| 28.750 | 0.0001299038711 | 400 | 0.10560 | 0.89440 | Yes |
| 22.860 | 0.0001579529300 | 400 | 0.10560 | 0.89440 | Yes |
| 17.385 | 0.0002020202020 | 400 | 0.10560 | 0.89440 | Yes |
| 11.889 | 0.0002887669651 | 400 | 0.10560 | 0.89440 | Yes |
| 5.747 | 0.0005854800937 | 400 | 0.10560 | 0.89440 | Yes |
| 68.727 | 0.0000675858340 | 400 | 0.25147 | 0.74853 | Yes |
| 63.061 | 0.0000709975151 | 400 | 0.25147 | 0.74853 | Yes |
| 57.436 | 0.0000750976269 | 400 | 0.25147 | 0.74853 | Yes |
| 51.693 | 0.0000802954874 | 400 | 0.25147 | 0.74853 | Yes |
| 45.922 | 0.0000869489610 | 400 | 0.25147 | 0.74853 | Yes |
| 40.281 | 0.0000955109838 | 400 | 0.25147 | 0.74853 | Yes |
| 34.456 | 0.0001075384450 | 400 | 0.25147 | 0.74853 | Yes |
| 28.669 | 0.0001249063203 | 400 | 0.25147 | 0.74853 | Yes |
| 23.064 | 0.0001507386192 | 400 | 0.25147 | 0.74853 | Yes |
| 16.675 | 0.0002033346889 | 400 | 0.25147 | 0.74853 | Yes |
| 11.547 | 0.0002894356006 | 400 | 0.25147 | 0.74853 | Yes |
| 5.867 | 0.0005659309564 | 400 | 0.25147 | 0.74853 | Yes |
| 68.619 | 0.0000627234523 | 400 | 0.50365 | 0.49635 | Yes |
| 63.139 | 0.0000654835964 | 400 | 0.50365 | 0.49635 | Yes |
| 57.289 | 0.0000690941754 | 400 | 0.50365 | 0.49635 | Yes |
| 51.725 | 0.0000733944954 | 400 | 0.50365 | 0.49635 | Yes |
| 45.830 | 0.0000792707095 | 400 | 0.50365 | 0.49635 | Yes |
| 40.049 | 0.0000870322019 | 400 | 0.50365 | 0.49635 | Yes |
| 34.424 | 0.0000975419430 | 400 | 0.50365 | 0.49635 | Yes |
| 28.635 | 0.0001135460429 | 400 | 0.50365 | 0.49635 | Yes |
| 22.930 | 0.0001386577926 | 400 | 0.50365 | 0.49635 | Yes |
| 17.447 | 0.0001805380032 | 400 | 0.50365 | 0.49635 | Yes |
| 11.530 | 0.0002746498215 | 400 | 0.50365 | 0.49635 | Yes |
| 6.060 | 0.0005307855626 | 400 | 0.50365 | 0.49635 | Yes |
| 68.723 | 0.0000584043920 | 400 | 0.71105 | 0.28895 | Yes |
| 63.024 | 0.0000607348922 | 400 | 0.71105 | 0.28895 | Yes |
| 57.544 | 0.0000634880325 | 400 | 0.71105 | 0.28895 | Yes |
| 51.834 | 0.0000670735797 | 400 | 0.71105 | 0.28895 | Yes |
| 45.987 | 0.0000718648940 | 400 | 0.71105 | 0.28895 | Yes |
| 40.123 | 0.0000784375245 | 400 | 0.71105 | 0.28895 | Yes |
| 34.480 | 0.0000874737579 | 400 | 0.71105 | 0.28895 | Yes |
| 28.678 | 0.0001016983627 | 400 | 0.71105 | 0.28895 | Yes |
| 22.998 | 0.0001247972045 | 400 | 0.71105 | 0.28895 | Yes |
| 17.097 | 0.0001691474966 | 400 | 0.71105 | 0.28895 | Yes |
| 11.537 | 0.0002586652871 | 400 | 0.71105 | 0.28895 | Yes |
| 5.890 | 0.0005316321106 | 400 | 0.71105 | 0.28895 | Yes |
| 68.626 | 0.0000543507799 | 400 | 0.90921 | 0.09079 | Yes |
| 63.073 | 0.0000560915414 | 400 | 0.90921 | 0.09079 | Yes |
| 57.472 | 0.0000582207732 | 400 | 0.90921 | 0.09079 | Yes |
| 51.935 | 0.0000608383525 | 400 | 0.90921 | 0.09079 | Yes |
| 45.955 | 0.0000645327827 | 400 | 0.90921 | 0.09079 | Yes |
| 40.612 | 0.0000689940665 | 400 | 0.90921 | 0.09079 | Yes |
| 34.588 | 0.0000763358779 | 400 | 0.90921 | 0.09079 | Yes |
| 28.277 | 0.0000891186169 | 400 | 0.90921 | 0.09079 | Yes |
| 23.033 | 0.0001080730574 | 400 | 0.90921 | 0.09079 | Yes |
| 17.344 | 0.0001478415139 | 400 | 0.90921 | 0.09079 | Yes |
| 11.728 | 0.0002345765893 | 400 | 0.90921 | 0.09079 | Yes |
| 6.627 | 0.0004508566276 | 400 | 0.90921 | 0.09079 | Yes |
| 68.588 | 0.0000773455024 | 450 | 0.10560 | 0.89440 | Yes |
| 57.394 | 0.0000867829558 | 450 | 0.10560 | 0.89440 | Yes |
| 51.431 | 0.0000935891437 | 450 | 0.10560 | 0.89440 | Yes |
| 45.745 | 0.0001018433649 | 450 | 0.10560 | 0.89440 | Yes |
| 40.044 | 0.0001125619090 | 450 | 0.10560 | 0.89440 | Yes |
| 34.451 | 0.0001266624446 | 450 | 0.10560 | 0.89440 | Yes |
| 28.416 | 0.0001485001485 | 450 | 0.10560 | 0.89440 | Yes |
| 22.867 | 0.0001791472590 | 450 | 0.10560 | 0.89440 | Yes |
| 17.279 | 0.0002306273063 | 450 | 0.10560 | 0.89440 | Yes |
| 11.263 | 0.0003447087211 | 450 | 0.10560 | 0.89440 | Yes |
| 5.828 | 0.0006527415144 | 450 | 0.10560 | 0.89440 | Yes |
| 68.690 | 0.0000749232037 | 450 | 0.25147 | 0.74853 | Yes |
| 63.105 | 0.0000789639924 | 450 | 0.25147 | 0.74853 | Yes |
| 57.351 | 0.0000840406757 | 450 | 0.25147 | 0.74853 | Yes |
| 51.698 | 0.0000901875902 | 450 | 0.25147 | 0.74853 | Yes |
| 45.871 | 0.0000982511299 | 450 | 0.25147 | 0.74853 | Yes |
| 40.112 | 0.0001086838387 | 450 | 0.25147 | 0.74853 | Yes |
| 34.454 | 0.0001225490196 | 450 | 0.25147 | 0.74853 | Yes |
| 28.331 | 0.0001443001443 | 450 | 0.25147 | 0.74853 | Yes |
| 23.239 | 0.0001717032967 | 450 | 0.25147 | 0.74853 | Yes |
| 17.196 | 0.0002262443439 | 450 | 0.25147 | 0.74853 | Yes |
| 11.652 | 0.0003278688525 | 450 | 0.25147 | 0.74853 | Yes |
| 5.613 | 0.0006711409396 | 450 | 0.25147 | 0.74853 | Yes |
| 68.770 | 0.0000702197879 | 450 | 0.50365 | 0.49635 | Yes |
| 63.009 | 0.0000739262216 | 450 | 0.50365 | 0.49635 | Yes |
| 57.446 | 0.0000782840144 | 450 | 0.50365 | 0.49635 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------------|-------------------|------------------|--------------------|
| 51.741 | 0.0000838926174 | 450 | 0.50365 | 0.49635 | Yes |
| 45.854 | 0.0000913242009 | 450 | 0.50365 | 0.49635 | Yes |
| 40.196 | 0.0001007759750 | 450 | 0.50365 | 0.49635 | Yes |
| 34.390 | 0.0001141552511 | 450 | 0.50365 | 0.49635 | Yes |
| 28.731 | 0.0001331026221 | 450 | 0.50365 | 0.49635 | Yes |
| 23.022 | 0.0001626545218 | 450 | 0.50365 | 0.49635 | Yes |
| 17.215 | 0.0002146383344 | 450 | 0.50365 | 0.49635 | Yes |
| 11.855 | 0.0003104625893 | 450 | 0.50365 | 0.49635 | Yes |
| 5.842 | 0.0006325110689 | 450 | 0.50365 | 0.49635 | Yes |
| 68.603 | 0.0000661157025 | 450 | 0.71105 | 0.28895 | Yes |
| 62.976 | 0.0000692712663 | 450 | 0.71105 | 0.28895 | Yes |
| 57.406 | 0.0000731101038 | 450 | 0.71105 | 0.28895 | Yes |
| 51.741 | 0.0000780274657 | 450 | 0.71105 | 0.28895 | Yes |
| 45.928 | 0.0000845522956 | 450 | 0.71105 | 0.28895 | Yes |
| 40.166 | 0.0000932835821 | 450 | 0.71105 | 0.28895 | Yes |
| 34.452 | 0.0001054296257 | 450 | 0.71105 | 0.28895 | Yes |
| 28.755 | 0.0001233654083 | 450 | 0.71105 | 0.28895 | Yes |
| 23.164 | 0.0001510345869 | 450 | 0.71105 | 0.28895 | Yes |
| 17.260 | 0.0002024701357 | 450 | 0.71105 | 0.28895 | Yes |
| 11.587 | 0.0003053435115 | 450 | 0.71105 | 0.28895 | Yes |
| 5.867 | 0.0006165228113 | 450 | 0.71105 | 0.28895 | Yes |
| 68.731 | 0.0000617932398 | 450 | 0.90921 | 0.09079 | Yes |
| 62.897 | 0.0000645078054 | 450 | 0.90921 | 0.09079 | Yes |
| 57.367 | 0.0000676910580 | 450 | 0.90921 | 0.09079 | Yes |
| 51.720 | 0.0000717978173 | 450 | 0.90921 | 0.09079 | Yes |
| 45.919 | 0.0000773514851 | 450 | 0.90921 | 0.09079 | Yes |
| 40.171 | 0.0000848824378 | 450 | 0.90921 | 0.09079 | Yes |
| 34.466 | 0.0000956480153 | 450 | 0.90921 | 0.09079 | Yes |
| 28.330 | 0.0001136880400 | 450 | 0.90921 | 0.09079 | Yes |
| 22.817 | 0.0001406271973 | 450 | 0.90921 | 0.09079 | Yes |
| 17.241 | 0.0001890001890 | 450 | 0.90921 | 0.09079 | Yes |
| 11.920 | 0.0002823263693 | 450 | 0.90921 | 0.09079 | Yes |
| 5.856 | 0.0006045949214 | 450 | 0.90921 | 0.09079 | Yes |

Continued: Data summarised from Table 1 of Brugge97 [86]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 69.031 | 5.03956E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 65.422 | 5.12952E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 62.028 | 5.22794E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 58.63 | 5.33874E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 55.214 | 5.46717E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 51.775 | 5.61293E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 48.387 | 5.77868E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 43.634 | 6.06134E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 39.295 | 6.38814E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 34.539 | 6.85965E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 30.092 | 7.25689E-05 | 300 | 0.3991 | 0.6009 | Yes |
| 69.189 | 4.638E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 57.633 | 4.88998E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 48.491 | 5.16983E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 41.194 | 5.48306E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 35.359 | 5.83533E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 30.659 | 6.23908E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 26.842 | 6.70376E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 23.732 | 7.23903E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 21.142 | 7.87092E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 18.932 | 8.62143E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 16.99 | 9.5429E-05 | 285 | 0.5037 | 0.4963 | Yes |
| 15.27 | 0.000106667 | 285 | 0.5037 | 0.4963 | Yes |
| 13.678 | 0.000120875 | 285 | 0.5037 | 0.4963 | Yes |
| 12.15 | 0.000139412 | 285 | 0.5037 | 0.4963 | Yes |
| 10.616 | 0.000165153 | 285 | 0.5037 | 0.4963 | Yes |
| 9.05 | 0.000202102 | 285 | 0.5037 | 0.4963 | Yes |
| 7.376 | 0.00026062 | 285 | 0.5037 | 0.4963 | Yes |
| 5.543 | 0.000366032 | 285 | 0.5037 | 0.4963 | Yes |
| 3.502 | 0.000614628 | 285 | 0.5037 | 0.4963 | Yes |
| 1.192 | 0.001915709 | 285 | 0.5037 | 0.4963 | Yes |
| 69.028 | 4.83863E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 58.681 | 5.10022E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 50.23 | 5.39345E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 43.426 | 5.71821E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 37.763 | 6.08828E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 33.118 | 6.50703E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 29.248 | 6.99203E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 26.056 | 7.54205E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 23.267 | 8.20008E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 20.829 | 8.99038E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 18.707 | 9.93147E-05 | 300 | 0.5037 | 0.4963 | Yes |
| 16.744 | 0.000111025 | 300 | 0.5037 | 0.4963 | Yes |
| 14.914 | 0.000125913 | 300 | 0.5037 | 0.4963 | Yes |
| 13.165 | 0.00014518 | 300 | 0.5037 | 0.4963 | Yes |
| 11.413 | 0.00017188 | 300 | 0.5037 | 0.4963 | Yes |
| 9.643 | 0.000210172 | 300 | 0.5037 | 0.4963 | Yes |

Data summarised from Table 1 of Duarte–Garza95–I [77]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 68.759 | 4.56163E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 62.510 | 4.69792E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 57.402 | 4.82952E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 51.819 | 5.0025E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 45.955 | 5.22575E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 40.271 | 5.50721E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 34.533 | 5.88998E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 28.832 | 6.45036E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 23.073 | 7.37409E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 17.334 | 9.14997E-05 | 225 | 0.10560 | 0.89440 | Yes |
| 11.565 | 0.000135044 | 225 | 0.10560 | 0.89440 | Yes |
| 5.789 | 0.000288184 | 225 | 0.10560 | 0.89440 | Yes |
| 68.723 | 4.32807E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 63.995 | 4.40703E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 59.486 | 4.49156E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 54.635 | 4.59643E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 50.028 | 4.71165E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 45.559 | 4.84449E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 40.832 | 5.01354E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 36.052 | 5.22821E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 31.521 | 5.49571E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 26.560 | 5.90842E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 22.097 | 6.48256E-05 | 225 | 0.25147 | 0.74853 | Yes |
| 17.324 | 7.58265E-05 | 225 | 0.25147 | 0.74853 | Yes |

Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 68.757 | 3.96589E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 64.284 | 4.01027E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 59.971 | 4.05696E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 55.490 | 4.11049E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 51.251 | 4.16736E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 47.029 | 4.23048E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 42.734 | 4.30367E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 38.334 | 4.39039E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 33.940 | 4.49337E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 29.435 | 4.62385E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 25.084 | 4.78858E-05 | 225 | 0.50365 | 0.49635 | Yes |
| 68.765 | 3.73204E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 63.528 | 3.76478E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 58.351 | 3.79997E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 52.872 | 3.84054E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 47.575 | 3.88425E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 42.444 | 3.93113E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 37.012 | 3.98708E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 31.663 | 4.05022E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 26.429 | 4.12354E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 20.934 | 4.21799E-05 | 225 | 0.71105 | 0.28895 | Yes |
| 68.831 | 3.5624E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 63.930 | 3.58141E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 59.307 | 3.60075E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 54.341 | 3.62253E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 49.927 | 3.64352E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 44.731 | 3.66946E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 40.095 | 3.69399E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 34.971 | 3.72329E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 30.735 | 3.74925E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 25.841 | 3.78143E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 23.482 | 3.79853E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 15.997 | 3.85758E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 11.238 | 3.90076E-05 | 225 | 0.90921 | 0.09079 | Yes |
| 68.953 | 4.81904E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 57.208 | 5.15597E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 49.629 | 5.45703E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 40.517 | 5.97514E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 34.424 | 6.49604E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 29.447 | 7.10934E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 25.196 | 7.87278E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 21.643 | 8.80592E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 18.586 | 9.97805E-05 | 245 | 0.10560 | 0.89440 | Yes |
| 15.875 | 0.000114969 | 245 | 0.10560 | 0.89440 | Yes |
| 13.324 | 0.000136221 | 245 | 0.10560 | 0.89440 | Yes |
| 10.939 | 0.000166556 | 245 | 0.10560 | 0.89440 | Yes |
| 8.579 | 0.000215193 | 245 | 0.10560 | 0.89440 | Yes |
| 6.223 | 0.000302847 | 245 | 0.10560 | 0.89440 | Yes |
| 3.806 | 0.000508388 | 245 | 0.10560 | 0.89440 | Yes |
| 1.265 | 0.001584786 | 245 | 0.10560 | 0.89440 | Yes |
| 68.896 | 4.56976E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 55.480 | 4.88377E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 45.088 | 5.24852E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 37.041 | 5.67634E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 30.934 | 6.16979E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 26.204 | 6.75128E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 22.498 | 7.43937E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 19.130 | 8.38785E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 16.575 | 9.49127E-05 | 245 | 0.25147 | 0.74853 | Yes |
| 14.379 | 0.000108909 | 245 | 0.25147 | 0.74853 | Yes |
| 12.171 | 0.000129971 | 245 | 0.25147 | 0.74853 | Yes |
| 10.182 | 0.00015916 | 245 | 0.25147 | 0.74853 | Yes |
| 8.167 | 0.000205846 | 245 | 0.25147 | 0.74853 | Yes |
| 6.057 | 0.000290782 | 245 | 0.25147 | 0.74853 | Yes |
| 3.737 | 0.000498753 | 245 | 0.25147 | 0.74853 | Yes |
| 1.182 | 0.001683502 | 245 | 0.25147 | 0.74853 | Yes |
| 69.031 | 4.17415E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 64.442 | 4.23173E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 59.570 | 4.30089E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 54.654 | 4.37848E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 49.798 | 4.46748E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 44.823 | 4.57498E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 40.137 | 4.69528E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 35.095 | 4.85625E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 30.213 | 5.0597E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 25.376 | 5.34017E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 20.573 | 5.77801E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 20.573 | 5.77801E-05 | 245 | 0.50365 | 0.49635 | Yes |
| 69.042 | 3.90976E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 64.182 | 3.94836E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 58.841 | 3.99457E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 56.941 | 4.03193E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 49.385 | 4.09149E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 44.239 | 4.15386E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 39.256 | 4.22279E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 34.043 | 4.30719E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 29.624 | 4.39309E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 24.157 | 4.52571E-05 | 245 | 0.71105 | 0.28895 | Yes |
| 18.997 | 4.69682E-05 | 245 | 0.71105 | 0.28895 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 68.926 | 3.71388E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 63.374 | 3.74223E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 57.687 | 3.77287E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 52.013 | 3.80691E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 46.110 | 3.84512E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 40.397 | 3.88682E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 34.971 | 3.92989E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 29.357 | 3.9801E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 23.315 | 4.04236E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 17.497 | 4.11336E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 11.846 | 4.19692E-05 | 245 | 0.90921 | 0.09079 | Yes |
| 68.418 | 4.29516E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 63.922 | 4.35996E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 59.345 | 4.43361E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 55.723 | 4.49924E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 50.245 | 4.61255E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 45.746 | 4.72077E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 41.210 | 4.85343E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 36.441 | 5.02462E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 32.023 | 5.22794E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 27.634 | 5.50025E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 22.818 | 5.94707E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 18.165 | 6.71006E-05 | 255 | 0.50365 | 0.49635 | Yes |
| 68.980 | 5.08751E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 59.626 | 5.39171E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 51.662 | 5.74119E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 45.014 | 6.13346E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 39.419 | 6.57722E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 34.460 | 7.10783E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 30.257 | 7.71843E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 26.580 | 8.44737E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 23.281 | 9.33881E-05 | 265 | 0.10560 | 0.89440 | Yes |
| 20.372 | 0.000104178 | 265 | 0.10560 | 0.89440 | Yes |
| 17.697 | 0.000117869 | 265 | 0.10560 | 0.89440 | Yes |
| 15.189 | 0.000135943 | 265 | 0.10560 | 0.89440 | Yes |
| 12.832 | 0.000160256 | 265 | 0.10560 | 0.89440 | Yes |
| 10.538 | 0.000195427 | 265 | 0.10560 | 0.89440 | Yes |
| 8.288 | 0.00025025 | 265 | 0.10560 | 0.89440 | Yes |
| 6.015 | 0.000348797 | 265 | 0.10560 | 0.89440 | Yes |
| 3.740 | 0.000570125 | 265 | 0.10560 | 0.89440 | Yes |
| 1.408 | 0.001545595 | 265 | 0.10560 | 0.89440 | Yes |
| 68.657 | 4.83676E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 58.009 | 5.1311E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 49.373 | 5.46179E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 42.394 | 5.8326E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 36.542 | 6.26841E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 31.649 | 6.77874E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 27.743 | 7.3497E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 24.334 | 8.0457E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 21.323 | 8.90551E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 18.758 | 9.93049E-05 | 265 | 0.25147 | 0.74853 | Yes |
| 16.383 | 0.0001126 | 265 | 0.25147 | 0.74853 | Yes |
| 14.202 | 0.000129955 | 265 | 0.25147 | 0.74853 | Yes |
| 12.108 | 0.00015387 | 265 | 0.25147 | 0.74853 | Yes |
| 10.005 | 0.00018843 | 265 | 0.25147 | 0.74853 | Yes |
| 8.034 | 0.000241488 | 265 | 0.25147 | 0.74853 | Yes |
| 5.906 | 0.000338524 | 265 | 0.25147 | 0.74853 | Yes |
| 3.669 | 0.000564334 | 265 | 0.25147 | 0.74853 | Yes |
| 1.242 | 0.001736111 | 265 | 0.25147 | 0.74853 | Yes |
| 69.001 | 4.39967E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 55.649 | 4.63994E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 43.359 | 4.9724E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 35.192 | 5.31604E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 29.030 | 5.71265E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 24.410 | 6.17627E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 20.995 | 6.70556E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 18.245 | 7.36106E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 16.080 | 8.15328E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 14.235 | 9.17011E-05 | 265 | 0.50365 | 0.49635 | Yes |
| 12.784 | 0.000103445 | 265 | 0.50365 | 0.49635 | Yes |
| 11.373 | 0.00011989 | 265 | 0.50365 | 0.49635 | Yes |
| 10.049 | 0.000141884 | 265 | 0.50365 | 0.49635 | Yes |
| 8.649 | 0.00017449 | 265 | 0.50365 | 0.49635 | Yes |
| 7.181 | 0.000225836 | 265 | 0.50365 | 0.49635 | Yes |
| 5.511 | 0.000319285 | 265 | 0.50365 | 0.49635 | Yes |
| 3.500 | 0.000550661 | 265 | 0.50365 | 0.49635 | Yes |
| 1.140 | 0.001858736 | 265 | 0.50365 | 0.49635 | Yes |
| 68.931 | 4.10442E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 57.785 | 4.22726E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 48.415 | 4.35939E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 40.580 | 4.49984E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 34.035 | 4.65354E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 28.869 | 4.81186E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 24.672 | 4.98206E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 21.376 | 5.16129E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 18.559 | 5.36682E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 16.504 | 5.57507E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 14.781 | 5.81598E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 13.579 | 6.0507E-05 | 265 | 0.71105 | 0.28895 | Yes |
| 13.579 | 6.0507E-05 | 265 | 0.71105 | 0.28895 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 68.251 | 3.8844E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 61.833 | 3.9268E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 56.018 | 3.96999E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 50.756 | 4.013E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 45.612 | 4.05959E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 41.002 | 4.10509E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 36.809 | 4.15093E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 32.721 | 4.2015E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 29.107 | 4.25116E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 25.874 | 4.30108E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 22.907 | 4.35199E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 20.145 | 4.40606E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 17.673 | 4.4603E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 15.450 | 4.51528E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 13.391 | 4.57415E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 11.756 | 4.62727E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 9.953 | 4.69462E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 8.547 | 4.75511E-05 | 265 | 0.90921 | 0.09079 | Yes |
| 69.014 | 4.51692E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 55.386 | 4.79363E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 45.081 | 5.10334E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 37.149 | 5.45792E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 31.129 | 5.86373E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 26.449 | 6.33794E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 22.837 | 6.8937E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 19.987 | 7.5523E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 17.566 | 8.38856E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 15.661 | 9.35279E-05 | 275 | 0.50365 | 0.49635 | Yes |
| 13.921 | 0.000106202 | 275 | 0.50365 | 0.49635 | Yes |
| 12.286 | 0.000123487 | 275 | 0.50365 | 0.49635 | Yes |
| 10.850 | 0.000145159 | 275 | 0.50365 | 0.49635 | Yes |
| 9.299 | 0.00017819 | 275 | 0.50365 | 0.49635 | Yes |
| 7.643 | 0.00023084 | 275 | 0.50365 | 0.49635 | Yes |
| 5.790 | 0.000326477 | 275 | 0.50365 | 0.49635 | Yes |
| 3.684 | 0.000553403 | 275 | 0.50365 | 0.49635 | Yes |
| 1.152 | 0.001915709 | 275 | 0.50365 | 0.49635 | Yes |
| 68.988 | 4.20751E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 56.724 | 4.36338E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 46.572 | 4.53576E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 38.614 | 4.71809E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 32.303 | 4.91425E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 27.197 | 5.13268E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 23.293 | 5.36682E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 20.170 | 5.63126E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 17.915 | 5.90179E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 16.008 | 6.22704E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 14.525 | 6.58979E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 13.428 | 6.97058E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 12.490 | 7.42115E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 12.490 | 7.42115E-05 | 275 | 0.71105 | 0.28895 | Yes |
| 69.124 | 5.36021E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 61.286 | 5.64812E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 54.492 | 5.96801E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 48.534 | 6.32671E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 43.343 | 6.73038E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 38.736 | 7.18597E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 34.711 | 7.69882E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 30.952 | 8.31463E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 27.610 | 9.03261E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 24.590 | 9.87752E-05 | 285 | 0.10560 | 0.89440 | Yes |
| 21.802 | 0.000109039 | 285 | 0.10560 | 0.89440 | Yes |
| 19.227 | 0.000121551 | 285 | 0.10560 | 0.89440 | Yes |
| 16.819 | 0.00013725 | 285 | 0.10560 | 0.89440 | Yes |
| 14.481 | 0.000158078 | 285 | 0.10560 | 0.89440 | Yes |
| 12.256 | 0.000185943 | 285 | 0.10560 | 0.89440 | Yes |
| 10.090 | 0.000225581 | 285 | 0.10560 | 0.89440 | Yes |
| 7.932 | 0.000288018 | 285 | 0.10560 | 0.89440 | Yes |
| 5.792 | 0.000396197 | 285 | 0.10560 | 0.89440 | Yes |
| 3.650 | 0.000634518 | 285 | 0.10560 | 0.89440 | Yes |
| 1.477 | 0.001587302 | 285 | 0.10560 | 0.89440 | Yes |
| 69.088 | 5.0958E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 60.329 | 5.37057E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 52.977 | 5.67472E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 46.679 | 6.01504E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 41.260 | 6.40287E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 36.619 | 6.84041E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 32.596 | 7.34053E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 29.030 | 7.92959E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 25.912 | 8.6103E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 23.106 | 9.42418E-05 | 285 | 0.25147 | 0.74853 | Yes |
| 20.577 | 0.000103961 | 285 | 0.25147 | 0.74853 | Yes |
| 18.220 | 0.000116077 | 285 | 0.25147 | 0.74853 | Yes |
| 15.997 | 0.000131492 | 285 | 0.25147 | 0.74853 | Yes |
| 13.903 | 0.000151355 | 285 | 0.25147 | 0.74853 | Yes |
| 11.845 | 0.000178763 | 285 | 0.25147 | 0.74853 | Yes |
| 9.840 | 0.000217486 | 285 | 0.25147 | 0.74853 | Yes |
| 7.824 | 0.000277624 | 285 | 0.25147 | 0.74853 | Yes |
| 5.730 | 0.00038625 | 285 | 0.25147 | 0.74853 | Yes |
| 3.582 | 0.000632511 | 285 | 0.25147 | 0.74853 | Yes |
| 1.354 | 0.001712329 | 285 | 0.25147 | 0.74853 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 69.189 | 4.638E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 57.633 | 4.88998E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 48.491 | 5.16983E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 41.194 | 5.48306E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 35.359 | 5.83533E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 30.659 | 6.23908E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 26.842 | 6.70376E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 23.732 | 7.23903E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 21.142 | 7.87092E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 18.932 | 8.62143E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 16.990 | 9.5429E-05 | 285 | 0.50365 | 0.49635 | Yes |
| 15.270 | 0.000106667 | 285 | 0.50365 | 0.49635 | Yes |
| 13.678 | 0.000120875 | 285 | 0.50365 | 0.49635 | Yes |
| 12.150 | 0.000139412 | 285 | 0.50365 | 0.49635 | Yes |
| 10.616 | 0.000165153 | 285 | 0.50365 | 0.49635 | Yes |
| 9.050 | 0.000202102 | 285 | 0.50365 | 0.49635 | Yes |
| 7.376 | 0.00026062 | 285 | 0.50365 | 0.49635 | Yes |
| 5.543 | 0.000366032 | 285 | 0.50365 | 0.49635 | Yes |
| 3.502 | 0.000614628 | 285 | 0.50365 | 0.49635 | Yes |
| 1.192 | 0.001915709 | 285 | 0.50365 | 0.49635 | Yes |
| 69.080 | 4.31276E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 55.607 | 4.51019E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 44.919 | 4.73015E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 35.358 | 5.02008E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 26.656 | 5.4606E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 21.011 | 5.9848E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 17.501 | 6.58198E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 15.302 | 7.22804E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 13.685 | 7.99808E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 12.389 | 8.97263E-05 | 285 | 0.71105 | 0.28895 | Yes |
| 11.377 | 0.000101564 | 285 | 0.71105 | 0.28895 | Yes |
| 10.346 | 0.000117966 | 285 | 0.71105 | 0.28895 | Yes |
| 9.405 | 0.000139919 | 285 | 0.71105 | 0.28895 | Yes |
| 8.387 | 0.000172117 | 285 | 0.71105 | 0.28895 | Yes |
| 7.189 | 0.000222668 | 285 | 0.71105 | 0.28895 | Yes |
| 5.658 | 0.000316656 | 285 | 0.71105 | 0.28895 | Yes |
| 3.656 | 0.000551572 | 285 | 0.71105 | 0.28895 | Yes |
| 1.088 | 0.002083333 | 285 | 0.71105 | 0.28895 | Yes |
| 69.019 | 4.06141E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 57.355 | 4.16597E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 47.721 | 4.27387E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 39.762 | 4.38462E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 32.843 | 4.50511E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 27.142 | 4.63177E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 22.447 | 4.76622E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 18.648 | 4.90966E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 15.654 | 5.05996E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 13.219 | 5.22357E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 11.374 | 5.39724E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 10.034 | 5.57445E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 9.013 | 5.76568E-05 | 285 | 0.90921 | 0.09079 | Yes |
| 69.055 | 5.57538E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 61.675 | 5.8713E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 55.165 | 6.20424E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 49.506 | 6.57073E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 44.370 | 6.99007E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 39.817 | 7.46491E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 35.681 | 8.01539E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 31.967 | 8.64454E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 28.534 | 9.40026E-05 | 300 | 0.10560 | 0.89440 | Yes |
| 25.493 | 0.000102638 | 300 | 0.10560 | 0.89440 | Yes |
| 22.642 | 0.000113122 | 300 | 0.10560 | 0.89440 | Yes |
| 19.933 | 0.000126279 | 300 | 0.10560 | 0.89440 | Yes |
| 17.400 | 0.000142714 | 300 | 0.10560 | 0.89440 | Yes |
| 14.971 | 0.000164258 | 300 | 0.10560 | 0.89440 | Yes |
| 12.682 | 0.000192753 | 300 | 0.10560 | 0.89440 | Yes |
| 10.413 | 0.000234082 | 300 | 0.10560 | 0.89440 | Yes |
| 8.196 | 0.000297354 | 300 | 0.10560 | 0.89440 | Yes |
| 5.999 | 0.000407166 | 300 | 0.10560 | 0.89440 | Yes |
| 3.767 | 0.00065189 | 300 | 0.10560 | 0.89440 | Yes |
| 1.537 | 0.001612903 | 300 | 0.10560 | 0.89440 | Yes |
| 69.107 | 5.33646E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 60.931 | 5.6262E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 54.037 | 5.94248E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 48.072 | 6.29485E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 42.827 | 6.69792E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 38.228 | 7.1541E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 34.097 | 7.68876E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 30.514 | 8.296E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 27.285 | 9.00576E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 24.350 | 9.85999E-05 | 300 | 0.25147 | 0.74853 | Yes |
| 21.667 | 0.000108826 | 300 | 0.25147 | 0.74853 | Yes |
| 19.169 | 0.000121477 | 300 | 0.25147 | 0.74853 | Yes |
| 16.816 | 0.000137438 | 300 | 0.25147 | 0.74853 | Yes |
| 14.565 | 0.000158253 | 300 | 0.25147 | 0.74853 | Yes |
| 12.396 | 0.000186289 | 300 | 0.25147 | 0.74853 | Yes |
| 10.244 | 0.00022686 | 300 | 0.25147 | 0.74853 | Yes |
| 8.099 | 0.000290023 | 300 | 0.25147 | 0.74853 | Yes |
| 5.937 | 0.000400641 | 300 | 0.25147 | 0.74853 | Yes |
| 3.713 | 0.000652316 | 300 | 0.25147 | 0.74853 | Yes |
| 1.436 | 0.00172117 | 300 | 0.25147 | 0.74853 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 69.028 | 4.83863E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 58.681 | 5.10022E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 50.230 | 5.39345E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 43.426 | 5.71821E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 37.763 | 6.08828E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 33.118 | 6.50703E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 29.248 | 6.99203E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 26.056 | 7.54205E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 23.267 | 8.20008E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 20.829 | 8.99038E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 18.707 | 9.93147E-05 | 300 | 0.50365 | 0.49635 | Yes |
| 16.744 | 0.000111025 | 300 | 0.50365 | 0.49635 | Yes |
| 14.914 | 0.000125913 | 300 | 0.50365 | 0.49635 | Yes |
| 13.165 | 0.00014518 | 300 | 0.50365 | 0.49635 | Yes |
| 11.413 | 0.00017188 | 300 | 0.50365 | 0.49635 | Yes |
| 9.643 | 0.000210172 | 300 | 0.50365 | 0.49635 | Yes |
| 7.789 | 0.000270636 | 300 | 0.50365 | 0.49635 | Yes |
| 5.819 | 0.000378072 | 300 | 0.50365 | 0.49635 | Yes |
| 3.652 | 0.000633312 | 300 | 0.50365 | 0.49635 | Yes |
| 1.262 | 0.001937984 | 300 | 0.50365 | 0.49635 | Yes |
| 69.024 | 4.48652E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 55.166 | 4.73037E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 44.719 | 5.00175E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 36.720 | 5.30701E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 30.675 | 5.65419E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 26.095 | 6.04741E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 22.632 | 6.49815E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 19.974 | 7.01361E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 17.845 | 7.63884E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 16.111 | 8.38856E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 14.704 | 9.27214E-05 | 300 | 0.71105 | 0.28895 | Yes |
| 13.465 | 0.000103466 | 300 | 0.71105 | 0.28895 | Yes |
| 12.271 | 0.000117716 | 300 | 0.71105 | 0.28895 | Yes |
| 11.181 | 0.000135465 | 300 | 0.71105 | 0.28895 | Yes |
| 9.989 | 0.000161108 | 300 | 0.71105 | 0.28895 | Yes |
| 8.735 | 0.000197278 | 300 | 0.71105 | 0.28895 | Yes |
| 7.292 | 0.000255102 | 300 | 0.71105 | 0.28895 | Yes |
| 5.602 | 0.000360231 | 300 | 0.71105 | 0.28895 | Yes |
| 3.567 | 0.000617284 | 300 | 0.71105 | 0.28895 | Yes |
| 1.147 | 0.002105263 | 300 | 0.71105 | 0.28895 | Yes |
| 69.020 | 4.20486E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 55.550 | 4.35521E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 43.810 | 4.53371E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 34.664 | 4.72657E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 26.591 | 4.97785E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 19.704 | 5.33049E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 14.523 | 5.86235E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 11.758 | 6.52869E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 10.406 | 7.32118E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 9.571 | 8.4488E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 9.037 | 9.84737E-05 | 300 | 0.90921 | 0.09079 | Yes |
| 8.608 | 0.00011609 | 300 | 0.90921 | 0.09079 | Yes |
| 8.212 | 0.000137438 | 300 | 0.90921 | 0.09079 | Yes |
| 7.677 | 0.00016835 | 300 | 0.90921 | 0.09079 | Yes |
| 6.831 | 0.000220361 | 300 | 0.90921 | 0.09079 | Yes |
| 5.587 | 0.000313578 | 300 | 0.90921 | 0.09079 | Yes |
| 3.708 | 0.000550964 | 300 | 0.90921 | 0.09079 | Yes |
| 1.031 | 0.002309469 | 300 | 0.90921 | 0.09079 | Yes |
| 34.747 | 8.78657E-05 | 320 | 0.10560 | 0.89440 | Yes |
| 30.700 | 9.61076E-05 | 320 | 0.10560 | 0.89440 | Yes |
| 27.037 | 0.000106067 | 320 | 0.10560 | 0.89440 | Yes |
| 23.668 | 0.000118329 | 320 | 0.10560 | 0.89440 | Yes |
| 20.550 | 0.000133618 | 320 | 0.10560 | 0.89440 | Yes |
| 17.649 | 0.000153327 | 320 | 0.10560 | 0.89440 | Yes |
| 14.819 | 0.00018044 | 320 | 0.10560 | 0.89440 | Yes |
| 12.114 | 0.000218962 | 320 | 0.10560 | 0.89440 | Yes |
| 9.397 | 0.000281057 | 320 | 0.10560 | 0.89440 | Yes |
| 6.805 | 0.000387597 | 320 | 0.10560 | 0.89440 | Yes |
| 4.181 | 0.000631712 | 320 | 0.10560 | 0.89440 | Yes |
| 1.740 | 0.001519757 | 320 | 0.10560 | 0.89440 | Yes |
| 69.011 | 5.59003E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 61.506 | 5.88755E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 54.928 | 6.22432E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 50.951 | 6.47082E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 45.125 | 6.92377E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 39.687 | 7.48727E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 35.619 | 8.04052E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 32.020 | 8.65876E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 28.675 | 9.40734E-05 | 320 | 0.25147 | 0.74853 | Yes |
| 25.733 | 0.000102596 | 320 | 0.25147 | 0.74853 | Yes |
| 22.962 | 0.000112994 | 320 | 0.25147 | 0.74853 | Yes |
| 20.261 | 0.000126374 | 320 | 0.25147 | 0.74853 | Yes |
| 17.748 | 0.000142898 | 320 | 0.25147 | 0.74853 | Yes |
| 15.405 | 0.000163854 | 320 | 0.25147 | 0.74853 | Yes |
| 13.081 | 0.000192641 | 320 | 0.25147 | 0.74853 | Yes |
| 10.804 | 0.000233918 | 320 | 0.25147 | 0.74853 | Yes |
| 8.566 | 0.00029656 | 320 | 0.25147 | 0.74853 | Yes |
| 6.308 | 0.000406174 | 320 | 0.25147 | 0.74853 | Yes |
| 3.923 | 0.000660502 | 320 | 0.25147 | 0.74853 | Yes |
| 1.554 | 0.001697793 | 320 | 0.25147 | 0.74853 | Yes |
| 69.044 | 5.10334E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 59.508 | 5.38503E-05 | 320 | 0.50365 | 0.49635 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 51.900 | 5.69282E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 45.580 | 6.03464E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 40.180 | 6.42591E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 35.685 | 6.86436E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 31.758 | 7.37463E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 28.435 | 7.95862E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 25.458 | 8.65876E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 22.859 | 9.47777E-05 | 320 | 0.50365 | 0.49635 | Yes |
| 20.472 | 0.000104745 | 320 | 0.50365 | 0.49635 | Yes |
| 18.276 | 0.000117206 | 320 | 0.50365 | 0.49635 | Yes |
| 16.233 | 0.000132521 | 320 | 0.50365 | 0.49635 | Yes |
| 14.233 | 0.000152858 | 320 | 0.50365 | 0.49635 | Yes |
| 12.261 | 0.000180603 | 320 | 0.50365 | 0.49635 | Yes |
| 10.290 | 0.000220507 | 320 | 0.50365 | 0.49635 | Yes |
| 8.230 | 0.000283688 | 320 | 0.50365 | 0.49635 | Yes |
| 6.074 | 0.000397141 | 320 | 0.50365 | 0.49635 | Yes |
| 3.800 | 0.000658762 | 320 | 0.50365 | 0.49635 | Yes |
| 1.353 | 0.001930502 | 320 | 0.50365 | 0.49635 | Yes |
| 68.951 | 4.72903E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 56.959 | 4.98902E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 47.500 | 5.28346E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 40.063 | 5.61672E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 34.288 | 5.98946E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 29.742 | 6.41972E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 26.138 | 6.91324E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 23.221 | 7.48727E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 20.797 | 8.1646E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 18.747 | 8.98311E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 16.988 | 9.97506E-05 | 320 | 0.71105 | 0.28895 | Yes |
| 15.338 | 0.000112284 | 320 | 0.71105 | 0.28895 | Yes |
| 13.797 | 0.000128353 | 320 | 0.71105 | 0.28895 | Yes |
| 12.287 | 0.000149611 | 320 | 0.71105 | 0.28895 | Yes |
| 10.719 | 0.00017963 | 320 | 0.71105 | 0.28895 | Yes |
| 9.068 | 0.000224215 | 320 | 0.71105 | 0.28895 | Yes |
| 7.231 | 0.000299133 | 320 | 0.71105 | 0.28895 | Yes |
| 5.144 | 0.000448833 | 320 | 0.71105 | 0.28895 | Yes |
| 2.761 | 0.000898473 | 320 | 0.71105 | 0.28895 | Yes |
| 1.224 | 0.002118644 | 320 | 0.71105 | 0.28895 | Yes |
| 69.065 | 4.41423E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 55.533 | 4.60936E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 41.924 | 4.90148E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 31.439 | 5.27398E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 24.524 | 5.70353E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 19.987 | 6.20771E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 17.288 | 6.73764E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 15.306 | 7.41125E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 13.907 | 8.21288E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 12.841 | 9.1878E-05 | 320 | 0.90921 | 0.09079 | Yes |
| 11.919 | 0.000104428 | 320 | 0.90921 | 0.09079 | Yes |
| 11.058 | 0.000120861 | 320 | 0.90921 | 0.09079 | Yes |
| 10.159 | 0.000143369 | 320 | 0.90921 | 0.09079 | Yes |
| 9.113 | 0.00017646 | 320 | 0.90921 | 0.09079 | Yes |
| 7.881 | 0.000226398 | 320 | 0.90921 | 0.09079 | Yes |
| 6.126 | 0.000328623 | 320 | 0.90921 | 0.09079 | Yes |
| 3.955 | 0.000572738 | 320 | 0.90921 | 0.09079 | Yes |
| 1.111 | 0.002298851 | 320 | 0.90921 | 0.09079 | Yes |
| 69.189 | 6.27668E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 62.799 | 6.60939E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 57.018 | 6.97983E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 51.735 | 7.39645E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 46.821 | 7.87402E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 42.587 | 8.38434E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 38.449 | 8.99928E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 34.625 | 9.71062E-05 | 350 | 0.10560 | 0.89440 | Yes |
| 31.132 | 0.000105274 | 350 | 0.10560 | 0.89440 | Yes |
| 27.855 | 0.000115035 | 350 | 0.10560 | 0.89440 | Yes |
| 24.756 | 0.000126839 | 350 | 0.10560 | 0.89440 | Yes |
| 21.856 | 0.000141223 | 350 | 0.10560 | 0.89440 | Yes |
| 19.062 | 0.000159464 | 350 | 0.10560 | 0.89440 | Yes |
| 16.417 | 0.000182782 | 350 | 0.10560 | 0.89440 | Yes |
| 13.867 | 0.000214133 | 350 | 0.10560 | 0.89440 | Yes |
| 11.366 | 0.000259269 | 350 | 0.10560 | 0.89440 | Yes |
| 8.925 | 0.000328192 | 350 | 0.10560 | 0.89440 | Yes |
| 6.550 | 0.000445236 | 350 | 0.10560 | 0.89440 | Yes |
| 4.182 | 0.000694927 | 350 | 0.10560 | 0.89440 | Yes |
| 1.840 | 0.001574803 | 350 | 0.10560 | 0.89440 | Yes |
| 69.195 | 6.00925E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 62.429 | 6.32871E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 56.348 | 6.68539E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 50.943 | 7.08316E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 46.046 | 7.5358E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 41.551 | 8.05542E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 37.578 | 8.62887E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 33.822 | 9.31532E-05 | 350 | 0.25147 | 0.74853 | Yes |
| 30.428 | 0.000101061 | 350 | 0.25147 | 0.74853 | Yes |
| 27.254 | 0.000110509 | 350 | 0.25147 | 0.74853 | Yes |
| 24.223 | 0.000122115 | 350 | 0.25147 | 0.74853 | Yes |
| 21.446 | 0.00013598 | 350 | 0.25147 | 0.74853 | Yes |
| 18.790 | 0.000153539 | 350 | 0.25147 | 0.74853 | Yes |
| 16.208 | 0.000176647 | 350 | 0.25147 | 0.74853 | Yes |
| 13.711 | 0.000207727 | 350 | 0.25147 | 0.74853 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 11.296 | 0.000251572 | 350 | 0.25147 | 0.74853 | Yes |
| 8.875 | 0.000320616 | 350 | 0.25147 | 0.74853 | Yes |
| 6.486 | 0.00043956 | 350 | 0.25147 | 0.74853 | Yes |
| 4.097 | 0.000699301 | 350 | 0.25147 | 0.74853 | Yes |
| 1.687 | 0.001706485 | 350 | 0.25147 | 0.74853 | Yes |
| 69.156 | 5.51572E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 61.236 | 5.81058E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 54.438 | 6.13987E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 48.458 | 6.51806E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 43.405 | 6.93001E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 38.918 | 7.40796E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 34.980 | 7.94976E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 31.453 | 8.58369E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 28.285 | 9.32836E-05 | 350 | 0.50365 | 0.49635 | Yes |
| 25.426 | 0.00010203 | 350 | 0.50365 | 0.49635 | Yes |
| 22.752 | 0.000112727 | 350 | 0.50365 | 0.49635 | Yes |
| 20.228 | 0.000126103 | 350 | 0.50365 | 0.49635 | Yes |
| 17.857 | 0.000142755 | 350 | 0.50365 | 0.49635 | Yes |
| 15.571 | 0.000164393 | 350 | 0.50365 | 0.49635 | Yes |
| 13.325 | 0.000193911 | 350 | 0.50365 | 0.49635 | Yes |
| 11.077 | 0.000236463 | 350 | 0.50365 | 0.49635 | Yes |
| 8.801 | 0.000302939 | 350 | 0.50365 | 0.49635 | Yes |
| 6.454 | 0.000421941 | 350 | 0.50365 | 0.49635 | Yes |
| 4.034 | 0.000691563 | 350 | 0.50365 | 0.49635 | Yes |
| 1.476 | 0.001953125 | 350 | 0.50365 | 0.49635 | Yes |
| 69.088 | 5.11326E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 59.363 | 5.392E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 51.469 | 5.6993E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 45.039 | 6.03938E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 39.580 | 6.43459E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 35.089 | 6.87758E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 31.309 | 7.38552E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 28.076 | 7.97575E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 25.267 | 8.67303E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 22.802 | 9.49668E-05 | 350 | 0.71105 | 0.28895 | Yes |
| 20.562 | 0.000104998 | 350 | 0.71105 | 0.28895 | Yes |
| 18.453 | 0.000117689 | 350 | 0.71105 | 0.28895 | Yes |
| 16.502 | 0.000133333 | 350 | 0.71105 | 0.28895 | Yes |
| 14.597 | 0.000153704 | 350 | 0.71105 | 0.28895 | Yes |
| 12.664 | 0.000181884 | 350 | 0.71105 | 0.28895 | Yes |
| 10.712 | 0.000222173 | 350 | 0.71105 | 0.28895 | Yes |
| 8.374 | 0.000296824 | 350 | 0.71105 | 0.28895 | Yes |
| 6.421 | 0.000401606 | 350 | 0.71105 | 0.28895 | Yes |
| 3.980 | 0.000678426 | 350 | 0.71105 | 0.28895 | Yes |
| 1.333 | 0.002132196 | 350 | 0.71105 | 0.28895 | Yes |
| 69.093 | 4.76122E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 56.576 | 5.01807E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 46.868 | 5.30532E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 39.302 | 5.63253E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 33.571 | 5.99628E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 29.105 | 6.41396E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 25.639 | 6.8918E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 22.896 | 7.45268E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 20.684 | 8.10636E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 18.865 | 8.87705E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 17.249 | 9.82608E-05 | 350 | 0.90921 | 0.09079 | Yes |
| 15.798 | 0.000109926 | 350 | 0.90921 | 0.09079 | Yes |
| 14.396 | 0.000124953 | 350 | 0.90921 | 0.09079 | Yes |
| 13.019 | 0.000144634 | 350 | 0.90921 | 0.09079 | Yes |
| 11.601 | 0.000170969 | 350 | 0.90921 | 0.09079 | Yes |
| 10.053 | 0.000209512 | 350 | 0.90921 | 0.09079 | Yes |
| 8.306 | 0.00027115 | 350 | 0.90921 | 0.09079 | Yes |
| 6.290 | 0.000384911 | 350 | 0.90921 | 0.09079 | Yes |
| 3.957 | 0.000659196 | 350 | 0.90921 | 0.09079 | Yes |
| 1.220 | 0.002304147 | 350 | 0.90921 | 0.09079 | Yes |
| 68.655 | 7.01557E-05 | 400 | 0.10560 | 0.89440 | Yes |
| 63.076 | 7.37518E-05 | 400 | 0.10560 | 0.89440 | Yes |
| 57.528 | 7.80823E-05 | 400 | 0.10560 | 0.89440 | Yes |
| 51.633 | 8.37591E-05 | 400 | 0.10560 | 0.89440 | Yes |
| 45.922 | 9.07606E-05 | 400 | 0.10560 | 0.89440 | Yes |
| 40.264 | 9.97506E-05 | 400 | 0.10560 | 0.89440 | Yes |
| 34.122 | 0.000113161 | 400 | 0.10560 | 0.89440 | Yes |
| 28.750 | 0.000129904 | 400 | 0.10560 | 0.89440 | Yes |
| 22.860 | 0.000157953 | 400 | 0.10560 | 0.89440 | Yes |
| 17.385 | 0.00020202 | 400 | 0.10560 | 0.89440 | Yes |
| 11.889 | 0.000288767 | 400 | 0.10560 | 0.89440 | Yes |
| 5.747 | 0.00058548 | 400 | 0.10560 | 0.89440 | Yes |
| 68.727 | 6.75858E-05 | 400 | 0.25147 | 0.74853 | Yes |
| 63.061 | 7.09975E-05 | 400 | 0.25147 | 0.74853 | Yes |
| 57.436 | 7.50976E-05 | 400 | 0.25147 | 0.74853 | Yes |
| 51.693 | 8.02955E-05 | 400 | 0.25147 | 0.74853 | Yes |
| 45.922 | 8.6949E-05 | 400 | 0.25147 | 0.74853 | Yes |
| 40.281 | 9.5511E-05 | 400 | 0.25147 | 0.74853 | Yes |
| 34.456 | 0.000107538 | 400 | 0.25147 | 0.74853 | Yes |
| 28.669 | 0.000124906 | 400 | 0.25147 | 0.74853 | Yes |
| 23.064 | 0.000150739 | 400 | 0.25147 | 0.74853 | Yes |
| 16.675 | 0.000203335 | 400 | 0.25147 | 0.74853 | Yes |
| 11.547 | 0.000289436 | 400 | 0.25147 | 0.74853 | Yes |
| 5.867 | 0.000565931 | 400 | 0.25147 | 0.74853 | Yes |
| 68.619 | 6.27235E-05 | 400 | 0.50365 | 0.49635 | Yes |
| 63.139 | 6.54836E-05 | 400 | 0.50365 | 0.49635 | Yes |
| 57.289 | 6.90942E-05 | 400 | 0.50365 | 0.49635 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 51.725 | 7.33945E-05 | 400 | 0.50365 | 0.49635 | Yes |
| 45.830 | 7.92707E-05 | 400 | 0.50365 | 0.49635 | Yes |
| 40.049 | 8.70322E-05 | 400 | 0.50365 | 0.49635 | Yes |
| 34.424 | 9.75419E-05 | 400 | 0.50365 | 0.49635 | Yes |
| 28.635 | 0.000113546 | 400 | 0.50365 | 0.49635 | Yes |
| 22.930 | 0.000138658 | 400 | 0.50365 | 0.49635 | Yes |
| 17.447 | 0.000180538 | 400 | 0.50365 | 0.49635 | Yes |
| 11.530 | 0.00027465 | 400 | 0.50365 | 0.49635 | Yes |
| 6.060 | 0.000530786 | 400 | 0.50365 | 0.49635 | Yes |
| 68.723 | 5.84044E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 63.024 | 6.07349E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 57.544 | 6.3488E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 51.834 | 6.70736E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 45.987 | 7.18649E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 40.123 | 7.84375E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 34.480 | 8.74738E-05 | 400 | 0.71105 | 0.28895 | Yes |
| 28.678 | 0.000101698 | 400 | 0.71105 | 0.28895 | Yes |
| 22.998 | 0.000124797 | 400 | 0.71105 | 0.28895 | Yes |
| 17.097 | 0.000169147 | 400 | 0.71105 | 0.28895 | Yes |
| 11.537 | 0.000258665 | 400 | 0.71105 | 0.28895 | Yes |
| 5.890 | 0.000531632 | 400 | 0.71105 | 0.28895 | Yes |
| 68.626 | 5.43508E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 63.073 | 5.60915E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 57.472 | 5.82208E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 51.935 | 6.08384E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 45.955 | 6.45328E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 40.612 | 6.89845E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 34.588 | 7.63359E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 28.277 | 8.91186E-05 | 400 | 0.90921 | 0.09079 | Yes |
| 23.033 | 0.000108073 | 400 | 0.90921 | 0.09079 | Yes |
| 17.344 | 0.000147842 | 400 | 0.90921 | 0.09079 | Yes |
| 11.728 | 0.000234577 | 400 | 0.90921 | 0.09079 | Yes |
| 6.627 | 0.000430857 | 400 | 0.90921 | 0.09079 | Yes |
| 68.588 | 7.73455E-05 | 450 | 0.10560 | 0.89440 | Yes |
| 57.394 | 8.6783E-05 | 450 | 0.10560 | 0.89440 | Yes |
| 51.431 | 9.35891E-05 | 450 | 0.10560 | 0.89440 | Yes |
| 45.745 | 0.000101843 | 450 | 0.10560 | 0.89440 | Yes |
| 40.044 | 0.000112562 | 450 | 0.10560 | 0.89440 | Yes |
| 34.451 | 0.000126662 | 450 | 0.10560 | 0.89440 | Yes |
| 28.416 | 0.0001485 | 450 | 0.10560 | 0.89440 | Yes |
| 22.867 | 0.000179147 | 450 | 0.10560 | 0.89440 | Yes |
| 17.279 | 0.000230627 | 450 | 0.10560 | 0.89440 | Yes |
| 11.263 | 0.000344709 | 450 | 0.10560 | 0.89440 | Yes |
| 5.828 | 0.000652742 | 450 | 0.10560 | 0.89440 | Yes |
| 68.690 | 7.49232E-05 | 450 | 0.25147 | 0.74853 | Yes |
| 63.105 | 7.8964E-05 | 450 | 0.25147 | 0.74853 | Yes |
| 57.351 | 8.40407E-05 | 450 | 0.25147 | 0.74853 | Yes |
| 51.698 | 9.01876E-05 | 450 | 0.25147 | 0.74853 | Yes |
| 45.871 | 9.82511E-05 | 450 | 0.25147 | 0.74853 | Yes |
| 40.112 | 0.000108684 | 450 | 0.25147 | 0.74853 | Yes |
| 34.454 | 0.000122549 | 450 | 0.25147 | 0.74853 | Yes |
| 28.331 | 0.0001443 | 450 | 0.25147 | 0.74853 | Yes |
| 23.239 | 0.000171703 | 450 | 0.25147 | 0.74853 | Yes |
| 17.196 | 0.000226244 | 450 | 0.25147 | 0.74853 | Yes |
| 11.652 | 0.000327869 | 450 | 0.25147 | 0.74853 | Yes |
| 5.613 | 0.000671141 | 450 | 0.25147 | 0.74853 | Yes |
| 68.770 | 7.02198E-05 | 450 | 0.50365 | 0.49635 | Yes |
| 63.009 | 7.39262E-05 | 450 | 0.50365 | 0.49635 | Yes |
| 57.446 | 7.8284E-05 | 450 | 0.50365 | 0.49635 | Yes |
| 51.741 | 8.38926E-05 | 450 | 0.50365 | 0.49635 | Yes |
| 45.854 | 9.13242E-05 | 450 | 0.50365 | 0.49635 | Yes |
| 40.196 | 0.000100776 | 450 | 0.50365 | 0.49635 | Yes |
| 34.390 | 0.000114155 | 450 | 0.50365 | 0.49635 | Yes |
| 28.731 | 0.000133103 | 450 | 0.50365 | 0.49635 | Yes |
| 23.022 | 0.000162655 | 450 | 0.50365 | 0.49635 | Yes |
| 17.215 | 0.000214638 | 450 | 0.50365 | 0.49635 | Yes |
| 11.855 | 0.000310463 | 450 | 0.50365 | 0.49635 | Yes |
| 5.842 | 0.000632511 | 450 | 0.50365 | 0.49635 | Yes |
| 68.603 | 6.61157E-05 | 450 | 0.71105 | 0.28895 | Yes |
| 62.976 | 6.92713E-05 | 450 | 0.71105 | 0.28895 | Yes |
| 57.406 | 7.31101E-05 | 450 | 0.71105 | 0.28895 | Yes |
| 51.741 | 7.80275E-05 | 450 | 0.71105 | 0.28895 | Yes |
| 45.928 | 8.45523E-05 | 450 | 0.71105 | 0.28895 | Yes |
| 40.166 | 9.32836E-05 | 450 | 0.71105 | 0.28895 | Yes |
| 34.452 | 0.00010543 | 450 | 0.71105 | 0.28895 | Yes |
| 28.755 | 0.000123365 | 450 | 0.71105 | 0.28895 | Yes |
| 23.164 | 0.000151035 | 450 | 0.71105 | 0.28895 | Yes |
| 17.260 | 0.00020247 | 450 | 0.71105 | 0.28895 | Yes |
| 11.587 | 0.000305344 | 450 | 0.71105 | 0.28895 | Yes |
| 5.867 | 0.000616523 | 450 | 0.71105 | 0.28895 | Yes |
| 68.731 | 6.17932E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 62.897 | 6.45078E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 57.367 | 6.76911E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 51.720 | 7.17978E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 45.919 | 7.73515E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 40.171 | 8.48824E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 34.466 | 9.5648E-05 | 450 | 0.90921 | 0.09079 | Yes |
| 28.330 | 0.000113688 | 450 | 0.90921 | 0.09079 | Yes |
| 22.817 | 0.000140627 | 450 | 0.90921 | 0.09079 | Yes |
| 17.241 | 0.000189 | 450 | 0.90921 | 0.09079 | Yes |
| 11.920 | 0.000282326 | 450 | 0.90921 | 0.09079 | Yes |
| 5.856 | 0.000604595 | 450 | 0.90921 | 0.09079 | Yes |

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | Usable Data Point? |
|------------|-------------------------------------|---------------|-------------------|------------------|--------------------|
| 7.5075386 | 4.163419E-05 | 250 | 0.982 | 0.018 | Yes |
| 16.8021364 | 4.191016E-05 | 260 | 0.982 | 0.018 | Yes |
| 8.6841811 | 4.551281E-05 | 270 | 0.982 | 0.018 | Yes |
| 26.9498034 | 4.201476E-05 | 270 | 0.982 | 0.018 | Yes |
| 32.0556331 | 4.205123E-05 | 275 | 0.982 | 0.018 | Yes |
| 16.0366138 | 4.579484E-05 | 280 | 0.982 | 0.018 | Yes |
| 9.1347922 | 4.994448E-05 | 285 | 0.982 | 0.018 | Yes |
| 12.0067428 | 5.009951E-05 | 290 | 0.982 | 0.018 | Yes |
| 23.8272641 | 4.591001E-05 | 290 | 0.982 | 0.018 | Yes |
| 8.7895674 | 5.540408E-05 | 295 | 0.982 | 0.018 | Yes |
| 5.1465335 | 3.329160E-04 | 300 | 0.982 | 0.018 | Yes |
| 11.0317251 | 5.554229E-05 | 300 | 0.982 | 0.018 | Yes |
| 17.9089753 | 5.031430E-05 | 300 | 0.982 | 0.018 | Yes |
| 31.6712158 | 4.598582E-05 | 300 | 0.982 | 0.018 | Yes |
| 2.2563767 | 1.001295E-03 | 305 | 0.982 | 0.018 | Yes |
| 6.9332505 | 1.994778E-04 | 305 | 0.982 | 0.018 | Yes |
| 6.9344043 | 1.995055E-04 | 305 | 0.982 | 0.018 | Yes |
| 7.6234034 | 1.427596E-04 | 305 | 0.982 | 0.018 | Yes |
| 9.7177665 | 6.281127E-05 | 305 | 0.982 | 0.018 | Yes |
| 13.2691923 | 5.568125E-05 | 305 | 0.982 | 0.018 | Yes |
| 2.3030787 | 1.001845E-03 | 310 | 0.982 | 0.018 | Yes |
| 5.4990380 | 3.334137E-04 | 310 | 0.982 | 0.018 | Yes |
| 7.2767758 | 1.996719E-04 | 310 | 0.982 | 0.018 | Yes |
| 7.2784895 | 1.996996E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.1559388 | 1.429245E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.4027714 | 1.258409E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.6037832 | 1.119534E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.7748915 | 1.007028E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.9505344 | 9.142770E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.1510023 | 8.369819E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.4131032 | 7.737188E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.8060106 | 7.196761E-05 | 310 | 0.982 | 0.018 | Yes |
| 11.3995553 | 6.296163E-05 | 310 | 0.982 | 0.018 | Yes |
| 15.5331725 | 5.581194E-05 | 310 | 0.982 | 0.018 | Yes |
| 15.5459561 | 5.578811E-05 | 310 | 0.982 | 0.018 | Yes |
| 23.8315070 | 5.041402E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.0117425 | 1.260071E-04 | 315 | 0.982 | 0.018 | Yes |
| 9.3045870 | 1.121102E-04 | 315 | 0.982 | 0.018 | Yes |
| 9.5713644 | 1.008523E-04 | 315 | 0.982 | 0.018 | Yes |
| 9.8485366 | 9.157197E-05 | 315 | 0.982 | 0.018 | Yes |
| 10.1636378 | 8.384112E-05 | 315 | 0.982 | 0.018 | Yes |
| 10.5555296 | 7.751614E-05 | 315 | 0.982 | 0.018 | Yes |
| 11.1010267 | 7.212122E-05 | 315 | 0.982 | 0.018 | Yes |
| 13.0922670 | 6.312050E-05 | 315 | 0.982 | 0.018 | Yes |
| 17.8357655 | 5.588562E-05 | 315 | 0.982 | 0.018 | Yes |
| 17.8576940 | 5.585414E-05 | 315 | 0.982 | 0.018 | Yes |
| 26.9949116 | 5.045537E-05 | 315 | 0.982 | 0.018 | Yes |
| 2.3954203 | 1.002953E-03 | 320 | 0.982 | 0.018 | Yes |
| 5.8424573 | 3.339247E-04 | 320 | 0.982 | 0.018 | Yes |
| 7.9446804 | 2.000773E-04 | 320 | 0.982 | 0.018 | Yes |
| 7.9463864 | 2.001047E-04 | 320 | 0.982 | 0.018 | Yes |
| 9.1854392 | 1.432882E-04 | 320 | 0.982 | 0.018 | Yes |
| 9.6104091 | 1.261898E-04 | 320 | 0.982 | 0.018 | Yes |
| 9.9980651 | 1.122872E-04 | 320 | 0.982 | 0.018 | Yes |
| 10.3631781 | 1.010250E-04 | 320 | 0.982 | 0.018 | Yes |
| 10.7486806 | 9.174282E-05 | 320 | 0.982 | 0.018 | Yes |
| 11.1825192 | 8.401268E-05 | 320 | 0.982 | 0.018 | Yes |
| 11.7078025 | 7.768306E-05 | 320 | 0.982 | 0.018 | Yes |
| 12.4064600 | 7.229140E-05 | 320 | 0.982 | 0.018 | Yes |
| 14.8072431 | 6.323965E-05 | 320 | 0.982 | 0.018 | Yes |
| 20.1535098 | 5.594284E-05 | 320 | 0.982 | 0.018 | Yes |
| 20.1726324 | 5.591106E-05 | 320 | 0.982 | 0.018 | Yes |
| 30.0249795 | 5.049208E-05 | 320 | 0.982 | 0.018 | Yes |
| 33.0510853 | 5.052643E-05 | 325 | 0.982 | 0.018 | Yes |
| 2.4871487 | 1.004076E-03 | 330 | 0.982 | 0.018 | Yes |
| 6.1782653 | 3.344536E-04 | 330 | 0.982 | 0.018 | Yes |
| 8.5922178 | 2.005131E-04 | 330 | 0.982 | 0.018 | Yes |
| 8.5942598 | 2.005400E-04 | 330 | 0.982 | 0.018 | Yes |
| 10.1820483 | 1.437140E-04 | 330 | 0.982 | 0.018 | Yes |
| 10.7838284 | 1.266147E-04 | 330 | 0.982 | 0.018 | Yes |
| 11.3624320 | 1.127037E-04 | 330 | 0.982 | 0.018 | Yes |
| 11.9329135 | 1.014280E-04 | 330 | 0.982 | 0.018 | Yes |
| 12.5417041 | 9.212397E-05 | 330 | 0.982 | 0.018 | Yes |
| 13.2369688 | 8.436464E-05 | 330 | 0.982 | 0.018 | Yes |
| 14.0287225 | 7.799266E-05 | 330 | 0.982 | 0.018 | Yes |
| 15.0469659 | 7.255003E-05 | 330 | 0.982 | 0.018 | Yes |
| 18.2752200 | 6.339305E-05 | 330 | 0.982 | 0.018 | Yes |
| 24.8029975 | 5.603500E-05 | 330 | 0.982 | 0.018 | Yes |
| 24.8365755 | 5.600308E-05 | 330 | 0.982 | 0.018 | Yes |

Data summarised from Table 31 of Ely87 [75]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{N_2} | Usable Data Point? |
|------------|-------------------------------------|---------------|-------------------|------------------|--------------------|
| 7.5075386 | 4.163419E-05 | 250 | 0.982 | 0.018 | Yes |
| 16.8021364 | 4.191016E-05 | 260 | 0.982 | 0.018 | Yes |
| 8.6841811 | 4.551281E-05 | 270 | 0.982 | 0.018 | Yes |
| 26.9498034 | 4.201476E-05 | 270 | 0.982 | 0.018 | Yes |
| 32.0556331 | 4.205123E-05 | 275 | 0.982 | 0.018 | Yes |
| 16.0366138 | 4.579484E-05 | 280 | 0.982 | 0.018 | Yes |
| 9.1347922 | 4.994448E-05 | 285 | 0.982 | 0.018 | Yes |
| 12.0067428 | 5.009951E-05 | 290 | 0.982 | 0.018 | Yes |
| 23.8272641 | 4.591001E-05 | 290 | 0.982 | 0.018 | Yes |
| 8.7895674 | 5.540408E-05 | 295 | 0.982 | 0.018 | Yes |
| 5.1465335 | 3.329160E-04 | 300 | 0.982 | 0.018 | Yes |
| 11.0317251 | 5.554229E-05 | 300 | 0.982 | 0.018 | Yes |
| 17.9089753 | 5.031430E-05 | 300 | 0.982 | 0.018 | Yes |
| 31.6712158 | 4.598582E-05 | 300 | 0.982 | 0.018 | Yes |
| 2.2563767 | 1.001295E-03 | 305 | 0.982 | 0.018 | Yes |
| 6.9332505 | 1.994778E-04 | 305 | 0.982 | 0.018 | Yes |
| 6.9344043 | 1.995055E-04 | 305 | 0.982 | 0.018 | Yes |
| 7.6234034 | 1.427596E-04 | 305 | 0.982 | 0.018 | Yes |
| 9.7177665 | 6.281127E-05 | 305 | 0.982 | 0.018 | Yes |
| 13.2691923 | 5.568125E-05 | 305 | 0.982 | 0.018 | Yes |
| 2.3030787 | 1.001845E-03 | 310 | 0.982 | 0.018 | Yes |
| 5.4990380 | 3.334137E-04 | 310 | 0.982 | 0.018 | Yes |
| 7.2767758 | 1.996719E-04 | 310 | 0.982 | 0.018 | Yes |
| 7.2784895 | 1.996996E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.1559388 | 1.429245E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.4027714 | 1.258409E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.6037832 | 1.119534E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.7748915 | 1.007028E-04 | 310 | 0.982 | 0.018 | Yes |
| 8.9505344 | 9.142770E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.1510023 | 8.369819E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.4131032 | 7.737188E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.8060106 | 7.196761E-05 | 310 | 0.982 | 0.018 | Yes |
| 11.3995553 | 6.296163E-05 | 310 | 0.982 | 0.018 | Yes |
| 15.5331725 | 5.581194E-05 | 310 | 0.982 | 0.018 | Yes |
| 15.5459561 | 5.578811E-05 | 310 | 0.982 | 0.018 | Yes |
| 23.8315070 | 5.041402E-05 | 310 | 0.982 | 0.018 | Yes |
| 9.0117425 | 1.260071E-04 | 315 | 0.982 | 0.018 | Yes |
| 9.3045870 | 1.121102E-04 | 315 | 0.982 | 0.018 | Yes |
| 9.5713644 | 1.008523E-04 | 315 | 0.982 | 0.018 | Yes |
| 9.8485366 | 9.157197E-05 | 315 | 0.982 | 0.018 | Yes |
| 10.1636378 | 8.384112E-05 | 315 | 0.982 | 0.018 | Yes |
| 10.5555296 | 7.751614E-05 | 315 | 0.982 | 0.018 | Yes |
| 11.1010267 | 7.212122E-05 | 315 | 0.982 | 0.018 | Yes |
| 13.0922670 | 6.312050E-05 | 315 | 0.982 | 0.018 | Yes |
| 17.8357655 | 5.588562E-05 | 315 | 0.982 | 0.018 | Yes |
| 17.8576940 | 5.585414E-05 | 315 | 0.982 | 0.018 | Yes |
| 26.9949116 | 5.045537E-05 | 315 | 0.982 | 0.018 | Yes |
| 2.3954203 | 1.002953E-03 | 320 | 0.982 | 0.018 | Yes |
| 5.8424573 | 3.339247E-04 | 320 | 0.982 | 0.018 | Yes |
| 7.9446804 | 2.000773E-04 | 320 | 0.982 | 0.018 | Yes |
| 7.9463864 | 2.001047E-04 | 320 | 0.982 | 0.018 | Yes |
| 9.1854392 | 1.432882E-04 | 320 | 0.982 | 0.018 | Yes |
| 9.6104091 | 1.261898E-04 | 320 | 0.982 | 0.018 | Yes |
| 9.9980651 | 1.122872E-04 | 320 | 0.982 | 0.018 | Yes |
| 10.3631781 | 1.010250E-04 | 320 | 0.982 | 0.018 | Yes |
| 10.7486806 | 9.174282E-05 | 320 | 0.982 | 0.018 | Yes |
| 11.1825192 | 8.401268E-05 | 320 | 0.982 | 0.018 | Yes |
| 11.7078025 | 7.768306E-05 | 320 | 0.982 | 0.018 | Yes |
| 12.4064600 | 7.229140E-05 | 320 | 0.982 | 0.018 | Yes |
| 14.8072431 | 6.323965E-05 | 320 | 0.982 | 0.018 | Yes |
| 20.1535098 | 5.594284E-05 | 320 | 0.982 | 0.018 | Yes |
| 20.1726324 | 5.591106E-05 | 320 | 0.982 | 0.018 | Yes |
| 30.0249795 | 5.049208E-05 | 320 | 0.982 | 0.018 | Yes |
| 33.0510853 | 5.052643E-05 | 325 | 0.982 | 0.018 | Yes |
| 2.4871487 | 1.004076E-03 | 330 | 0.982 | 0.018 | Yes |
| 6.1782653 | 3.344536E-04 | 330 | 0.982 | 0.018 | Yes |
| 8.5922178 | 2.005131E-04 | 330 | 0.982 | 0.018 | Yes |
| 8.5942598 | 2.005400E-04 | 330 | 0.982 | 0.018 | Yes |
| 10.1820483 | 1.437140E-04 | 330 | 0.982 | 0.018 | Yes |
| 10.7838284 | 1.266147E-04 | 330 | 0.982 | 0.018 | Yes |
| 11.3624320 | 1.127037E-04 | 330 | 0.982 | 0.018 | Yes |
| 11.9329135 | 1.014280E-04 | 330 | 0.982 | 0.018 | Yes |
| 12.5417041 | 9.212397E-05 | 330 | 0.982 | 0.018 | Yes |
| 13.2369688 | 8.436464E-05 | 330 | 0.982 | 0.018 | Yes |
| 14.0287225 | 7.799266E-05 | 330 | 0.982 | 0.018 | Yes |
| 15.0469659 | 7.255003E-05 | 330 | 0.982 | 0.018 | Yes |
| 18.2752200 | 6.339305E-05 | 330 | 0.982 | 0.018 | Yes |
| 24.8029975 | 5.603500E-05 | 330 | 0.982 | 0.018 | Yes |
| 24.8365755 | 5.600308E-05 | 330 | 0.982 | 0.018 | Yes |

Data summarised from TABLE 1 of Ely89 [88]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 41.0044 | 6.06493E-05 | 300 | 0.44696 | 0.55304 | Yes |
| 27.6350 | 7.61709E-05 | 300 | 0.44696 | 0.55304 | Yes |
| 21.8676 | 9.1297E-05 | 300 | 0.44696 | 0.55304 | Yes |
| 17.1630 | 0.000114686 | 300 | 0.44696 | 0.55304 | Yes |
| 15.5039 | 0.000127457 | 300 | 0.44696 | 0.55304 | Yes |
| 14.4664 | 0.000137471 | 300 | 0.44696 | 0.55304 | Yes |
| 11.8033 | 0.000172698 | 300 | 0.44696 | 0.55304 | Yes |
| 10.7563 | 0.000191915 | 300 | 0.44696 | 0.55304 | Yes |
| 10.0742 | 0.000207011 | 300 | 0.44696 | 0.55304 | Yes |
| 8.2505 | 0.000260067 | 300 | 0.44696 | 0.55304 | Yes |
| 7.5166 | 0.000288968 | 300 | 0.44696 | 0.55304 | Yes |
| 7.0283 | 0.000311741 | 300 | 0.44696 | 0.55304 | Yes |
| 5.7271 | 0.000391646 | 300 | 0.44696 | 0.55304 | Yes |
| 5.1038 | 0.000443626 | 300 | 0.44696 | 0.55304 | Yes |
| 4.8546 | 0.000469476 | 300 | 0.44696 | 0.55304 | Yes |
| 3.9310 | 0.000589814 | 300 | 0.44696 | 0.55304 | Yes |
| 3.5629 | 0.000655139 | 300 | 0.44696 | 0.55304 | Yes |
| 3.3171 | 0.000707027 | 300 | 0.44696 | 0.55304 | Yes |
| 2.9142 | 0.000810839 | 300 | 0.44696 | 0.55304 | Yes |
| 2.6721 | 0.000888271 | 300 | 0.44696 | 0.55304 | Yes |
| 2.4173 | 0.000986571 | 300 | 0.44696 | 0.55304 | Yes |
| 1.9696 | 0.001221077 | 300 | 0.44696 | 0.55304 | Yes |
| 1.8035 | 0.001337754 | 300 | 0.44696 | 0.55304 | Yes |
| 1.6290 | 0.001485687 | 300 | 0.44696 | 0.55304 | Yes |
| 1.5126 | 0.001603617 | 300 | 0.44696 | 0.55304 | Yes |
| 1.3236 | 0.001839026 | 300 | 0.44696 | 0.55304 | Yes |
| 1.2109 | 0.002014708 | 300 | 0.44696 | 0.55304 | Yes |
| 1.0923 | 0.002237747 | 300 | 0.44696 | 0.55304 | Yes |
| 1.0157 | 0.00241038 | 300 | 0.44696 | 0.55304 | Yes |
| 1.0129 | 0.002415132 | 300 | 0.44696 | 0.55304 | Yes |
| 0.8860 | 0.002810681 | 300 | 0.44696 | 0.55304 | Yes |
| 0.8099 | 0.003034246 | 300 | 0.44696 | 0.55304 | Yes |
| 0.6776 | 0.003637306 | 300 | 0.44696 | 0.55304 | Yes |
| 0.5916 | 0.004171228 | 300 | 0.44696 | 0.55304 | Yes |
| 0.5405 | 0.004569744 | 300 | 0.44696 | 0.55304 | Yes |
| 0.4518 | 0.005477952 | 300 | 0.44696 | 0.55304 | Yes |
| 0.3942 | 0.006282211 | 300 | 0.44696 | 0.55304 | Yes |
| 0.3600 | 0.006882337 | 300 | 0.44696 | 0.55304 | Yes |
| 0.3009 | 0.008250169 | 300 | 0.44696 | 0.55304 | Yes |
| 0.2624 | 0.009460841 | 300 | 0.44696 | 0.55304 | Yes |
| 0.2396 | 0.01036523 | 300 | 0.44696 | 0.55304 | Yes |
| 0.2001 | 0.012425343 | 300 | 0.44696 | 0.55304 | Yes |
| 0.1745 | 0.01424923 | 300 | 0.44696 | 0.55304 | Yes |
| 0.1593 | 0.015610252 | 300 | 0.44696 | 0.55304 | Yes |
| 0.1330 | 0.018713486 | 300 | 0.44696 | 0.55304 | Yes |
| 0.1160 | 0.021455726 | 300 | 0.44696 | 0.55304 | Yes |
| 0.1059 | 0.023511005 | 300 | 0.44696 | 0.55304 | Yes |
| 0.0884 | 0.028184405 | 300 | 0.44696 | 0.55304 | Yes |

Data summarised from Table 2 of Esper89 [78]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 49.0 | 6.75395E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 50.0 | 6.68629E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 51.0 | 6.6186E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 52.0 | 6.55092E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 53.1 | 6.48199E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 54.1 | 6.4145E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 55.2 | 6.34714E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 56.4 | 6.27995E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 57.6 | 6.21175E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 58.9 | 6.14384E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 60.3 | 6.07625E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 61.6 | 6.00788E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 63.1 | 5.94102E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 64.7 | 5.87241E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 66.3 | 5.80536E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 68.0 | 5.73778E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 69.9 | 5.66973E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 71.7 | 5.60231E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 72.8 | 5.56823E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 73.7 | 5.54317E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 75.5 | 5.48621E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 77.4 | 5.43041E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 79.4 | 5.37393E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 81.5 | 5.31773E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 83.6 | 5.26183E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 86.0 | 5.20539E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 88.4 | 5.14933E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 90.9 | 5.09366E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 93.6 | 5.03679E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 96.5 | 4.98118E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 99.2 | 4.92452E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 102.4 | 4.86839E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 113.2 | 4.69982E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 117.3 | 4.64395E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 119.5 | 4.61585E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 121.7 | 4.56976E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 125.4 | 4.5233E-05 | 323 | 0.2515 | 0.7485 | Yes |

Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [119]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 129.5 | 4.47715E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 133.8 | 4.43071E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 138.2 | 4.38462E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 142.9 | 4.3383E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 147.8 | 4.2918E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 152.9 | 4.24516E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 158.4 | 4.19898E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 164.7 | 4.15271E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 170.9 | 4.1064E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 177.4 | 4.06008E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 184.3 | 4.01378E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 192.1 | 3.96706E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 200.0 | 3.92141E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 208.6 | 3.87492E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 217.8 | 3.82861E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 222.3 | 3.80542E-05 | 323 | 0.2515 | 0.7485 | Yes |
| 51.1 | 7.06528E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 52.0 | 6.99432E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 53.0 | 6.92328E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 54.0 | 6.85219E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 55.1 | 6.78112E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 56.1 | 6.7101E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 57.2 | 6.63917E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 58.3 | 6.56838E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 59.6 | 6.49777E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 60.8 | 6.42737E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 62.1 | 6.35595E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 63.4 | 6.28487E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 64.8 | 6.21416E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 66.3 | 6.14384E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 67.9 | 6.0728E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 69.5 | 6.00112E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 71.1 | 5.93112E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 73.0 | 5.85952E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 74.0 | 5.82436E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 75.9 | 5.75013E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 77.5 | 5.6919E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 79.3 | 5.63384E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 81.4 | 5.57598E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 83.5 | 5.5174E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 85.5 | 5.4591E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 87.8 | 5.40111E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 90.1 | 5.34256E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 92.7 | 5.28439E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 95.2 | 5.22577E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 98.0 | 5.16761E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 100.8 | 5.10991E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 103.8 | 5.05109E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 107.2 | 4.99283E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 110.8 | 4.93438E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 114.3 | 4.87654E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 118.2 | 4.81787E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 120.2 | 4.78906E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 122.5 | 4.74086E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 126.0 | 4.69294E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 129.9 | 4.64463E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 134.0 | 4.59664E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 138.2 | 4.54899E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 142.7 | 4.50105E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 147.4 | 4.45288E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 152.5 | 4.40451E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 157.7 | 4.35659E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 163.5 | 4.30854E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 169.4 | 4.26041E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 175.5 | 4.21278E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 182.4 | 4.16459E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 189.6 | 4.11642E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 197.3 | 4.06833E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 205.3 | 4.01983E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 214.0 | 3.97247E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 218.8 | 3.94848E-05 | 348 | 0.2515 | 0.7485 | Yes |
| 63.3 | 5.72977E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 64.8 | 5.67197E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 66.4 | 5.61447E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 68.2 | 5.55729E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 70.0 | 5.49963E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 72.0 | 5.44236E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 74.1 | 5.38549E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 76.3 | 5.32749E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 78.7 | 5.26999E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 81.2 | 5.21225E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 83.9 | 5.15504E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 86.8 | 5.09768E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 89.7 | 5.04021E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 92.9 | 4.98268E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 96.1 | 4.92514E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 103.7 | 4.81022E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 107.8 | 4.75291E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 109.8 | 4.72387E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 113.2 | 4.67624E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 117.2 | 4.62899E-05 | 323 | 0.5685 | 0.4315 | Yes |

Continued: Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [119]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 121.3 | 4.58212E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 125.8 | 4.53397E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 130.6 | 4.48736E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 135.7 | 4.43958E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 141.1 | 4.39228E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 146.7 | 4.34496E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 152.8 | 4.29766E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 159.3 | 4.24991E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 166.2 | 4.20274E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 173.5 | 4.15521E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 181.3 | 4.10783E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 189.7 | 4.01319E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 208.2 | 3.96559E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 218.6 | 3.91827E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 224.2 | 3.89483E-05 | 323 | 0.5685 | 0.4315 | Yes |
| 65.6 | 6.03448E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 67.1 | 5.97328E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 68.8 | 5.91331E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 70.6 | 5.85268E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 72.4 | 5.79238E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 74.3 | 5.73154E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 76.3 | 5.6711E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 78.4 | 5.61022E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 80.6 | 5.54981E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 83.1 | 5.48905E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 85.6 | 5.42882E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 88.2 | 5.36834E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 91.0 | 5.30768E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 94.0 | 5.24689E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 97.1 | 5.18675E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 100.5 | 5.12585E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 104.1 | 5.06567E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 107.9 | 5.00553E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 109.8 | 4.97466E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 113.0 | 4.92514E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 115.4 | 4.87531E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 120.4 | 4.82523E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 124.4 | 4.77493E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 128.8 | 4.72507E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 133.4 | 4.67566E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 138.3 | 4.62553E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 143.3 | 4.5759E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 148.7 | 4.52567E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 154.5 | 4.476E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 160.8 | 4.42581E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 167.3 | 4.37622E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 174.3 | 4.32622E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 181.6 | 4.27587E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 189.7 | 4.2262E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 198.2 | 4.17625E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 207.2 | 4.12656E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 212.2 | 4.10147E-05 | 348 | 0.5685 | 0.4315 | Yes |
| 56.4 | 5.29927E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 58.5 | 5.24566E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 60.3 | 5.24566E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 62.3 | 5.13966E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 64.6 | 5.08662E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 66.8 | 5.0334E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 69.2 | 4.98004E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 71.8 | 4.9272E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 74.6 | 4.87367E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 77.5 | 4.82072E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 80.7 | 4.76719E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 84.2 | 4.71429E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 87.9 | 4.66091E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 91.8 | 4.60766E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 96.0 | 4.55458E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 100.5 | 4.50169E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 105.5 | 4.44853E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 111.0 | 4.39516E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 113.9 | 4.36871E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 119.0 | 4.32517E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 124.1 | 4.28112E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 129.7 | 4.2375E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 135.9 | 4.19345E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 142.3 | 4.14943E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 149.2 | 4.10591E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 156.6 | 4.06205E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 164.5 | 4.01832E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 173.0 | 3.97432E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 182.2 | 3.9305E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 191.8 | 3.88651E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 202.3 | 3.84275E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 213.5 | 3.79888E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 224.1 | 3.75529E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 237.0 | 3.71131E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 250.8 | 3.66768E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 265.8 | 3.62374E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 273.7 | 3.60184E-05 | 323 | 0.7450 | 0.2550 | Yes |
| 60.6 | 5.52741E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 62.4 | 5.47211E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 64.3 | 5.41718E-05 | 348 | 0.7450 | 0.2550 | Yes |

Continued: Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [119]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 66.3 | 5.36117E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 68.2 | 5.30631E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 70.4 | 5.25049E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 72.3 | 5.19516E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 75.2 | 5.13966E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 77.9 | 5.08403E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 80.7 | 5.02897E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 83.8 | 4.97322E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 86.8 | 4.91809E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 90.3 | 4.8624E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 94.1 | 4.80679E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 97.9 | 4.75131E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 102.0 | 4.69599E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 106.6 | 4.64086E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 111.3 | 4.58491E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 113.9 | 4.55718E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 118.0 | 4.51186E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 122.7 | 4.46594E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 127.7 | 4.42046E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 132.9 | 4.37445E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 138.7 | 4.32892E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 144.7 | 4.28296E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 151.2 | 4.2375E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 158.0 | 4.19169E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 165.5 | 4.14599E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 173.3 | 4.10001E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 181.7 | 4.05463E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 190.7 | 4.00863E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 200.2 | 3.96288E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 210.7 | 3.91739E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 221.9 | 3.87181E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 233.8 | 3.82581E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 246.3 | 3.78018E-05 | 348 | 0.7450 | 0.2550 | Yes |
| 252.7 | 3.75741E-05 | 348 | 0.7450 | 0.2550 | Yes |

Continued: Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [108]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 3.03975 | 0.000760956 | 298.15 | 0.5048 | 0.4952 | Yes |
| 5.06625 | 0.000435631 | 298.15 | 0.5048 | 0.4952 | Yes |
| 7.59938 | 0.00027411 | 298.15 | 0.5048 | 0.4952 | Yes |
| 10.13250 | 0.000194842 | 298.15 | 0.5048 | 0.4952 | Yes |
| 12.66563 | 0.000149219 | 298.15 | 0.5048 | 0.4952 | Yes |
| 15.19875 | 0.000120908 | 298.15 | 0.5048 | 0.4952 | Yes |
| 17.73188 | 0.000102615 | 298.15 | 0.5048 | 0.4952 | Yes |
| 20.26500 | 9.05587E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 22.79813 | 8.19102E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 25.33125 | 7.55002E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 30.39750 | 6.74348E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 35.46375 | 6.20582E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 40.53000 | 5.82949E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 45.59625 | 5.54767E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 50.66250 | 5.32416E-05 | 298.15 | 0.5048 | 0.4952 | Yes |
| 3.03975 | 0.000790722 | 298.15 | 0.2513 | 0.7487 | Yes |
| 5.06625 | 0.000466017 | 298.15 | 0.2513 | 0.7487 | Yes |
| 7.59938 | 0.000304969 | 298.15 | 0.2513 | 0.7487 | Yes |
| 10.13250 | 0.00022562 | 298.15 | 0.2513 | 0.7487 | Yes |
| 12.66563 | 0.000179067 | 298.15 | 0.2513 | 0.7487 | Yes |
| 15.19875 | 0.000149761 | 298.15 | 0.2513 | 0.7487 | Yes |
| 17.73188 | 0.000128255 | 298.15 | 0.2513 | 0.7487 | Yes |
| 20.26500 | 0.000113385 | 298.15 | 0.2513 | 0.7487 | Yes |
| 22.79813 | 0.000102309 | 298.15 | 0.2513 | 0.7487 | Yes |
| 25.33125 | 9.37808E-05 | 298.15 | 0.2513 | 0.7487 | Yes |
| 30.39750 | 8.1641E-05 | 298.15 | 0.2513 | 0.7487 | Yes |
| 35.46375 | 7.37178E-05 | 298.15 | 0.2513 | 0.7487 | Yes |
| 40.53000 | 6.81361E-05 | 298.15 | 0.2513 | 0.7487 | Yes |
| 45.59625 | 6.38384E-05 | 298.15 | 0.2513 | 0.7487 | Yes |
| 50.66250 | 6.05372E-05 | 298.15 | 0.2513 | 0.7487 | Yes |
| 3.03975 | 0.000711345 | 273.15 | 0.5048 | 0.4952 | Yes |
| 5.06625 | 0.000413583 | 273.15 | 0.5048 | 0.4952 | Yes |
| 7.59938 | 0.00026562 | 273.15 | 0.5048 | 0.4952 | Yes |
| 10.13250 | 0.000192603 | 273.15 | 0.5048 | 0.4952 | Yes |
| 12.66563 | 0.000149905 | 273.15 | 0.5048 | 0.4952 | Yes |
| 15.19875 | 0.000122545 | 273.15 | 0.5048 | 0.4952 | Yes |
| 17.73188 | 0.000104142 | 273.15 | 0.5048 | 0.4952 | Yes |
| 20.26500 | 9.13481E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 22.79813 | 8.19654E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 25.33125 | 7.49523E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 30.39750 | 6.52844E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 35.46375 | 5.92113E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 40.53000 | 5.48414E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 45.59625 | 5.16517E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 50.66250 | 4.93152E-05 | 273.15 | 0.5048 | 0.4952 | Yes |

Data summarised from TABLE II of Haney44 [108]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 3.03975 | 0.000732563 | 273.15 | 0.2513 | 0.7487 | Yes |
| 5.06625 | 0.000434741 | 273.15 | 0.2513 | 0.7487 | Yes |
| 7.59938 | 0.00028669 | 273.15 | 0.2513 | 0.7487 | Yes |
| 10.13250 | 0.000213538 | 273.15 | 0.2513 | 0.7487 | Yes |
| 12.66563 | 0.000170292 | 273.15 | 0.2513 | 0.7487 | Yes |
| 15.19875 | 0.00014206 | 273.15 | 0.2513 | 0.7487 | Yes |
| 17.73188 | 0.00012247 | 273.15 | 0.2513 | 0.7487 | Yes |
| 20.26500 | 0.000107161 | 273.15 | 0.2513 | 0.7487 | Yes |
| 22.79813 | 9.74858E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 25.33125 | 8.91538E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 30.39750 | 7.71041E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 35.46375 | 6.89198E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 40.53000 | 6.31345E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 45.59625 | 5.89388E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 50.66250 | 5.54656E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 3.03975 | 0.000721431 | 273.15 | 0.5048 | 0.4952 | Yes |
| 5.06625 | 0.000423445 | 273.15 | 0.5048 | 0.4952 | Yes |
| 7.59938 | 0.000275244 | 273.15 | 0.5048 | 0.4952 | Yes |
| 10.13250 | 0.000201995 | 273.15 | 0.5048 | 0.4952 | Yes |
| 12.66563 | 0.00015887 | 273.15 | 0.5048 | 0.4952 | Yes |
| 15.19875 | 0.000130927 | 273.15 | 0.5048 | 0.4952 | Yes |
| 17.73188 | 0.000111711 | 273.15 | 0.5048 | 0.4952 | Yes |
| 20.26500 | 9.77921E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 22.79813 | 8.74244E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 25.33125 | 7.95337E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 30.39750 | 6.85419E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 35.46375 | 6.13502E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 40.53000 | 5.62535E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 45.59625 | 5.25383E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 50.66250 | 4.98487E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 3.03975 | 0.000737718 | 273.15 | 0.2513 | 0.7487 | Yes |
| 5.06625 | 0.000439941 | 273.15 | 0.2513 | 0.7487 | Yes |
| 7.59938 | 0.000291591 | 273.15 | 0.2513 | 0.7487 | Yes |
| 10.13250 | 0.000218178 | 273.15 | 0.2513 | 0.7487 | Yes |
| 12.66563 | 0.000174703 | 273.15 | 0.2513 | 0.7487 | Yes |
| 15.19875 | 0.000146169 | 273.15 | 0.2513 | 0.7487 | Yes |
| 17.73188 | 0.000126197 | 273.15 | 0.2513 | 0.7487 | Yes |
| 20.26500 | 0.00011532 | 273.15 | 0.2513 | 0.7487 | Yes |
| 22.79813 | 0.000100325 | 273.15 | 0.2513 | 0.7487 | Yes |
| 25.33125 | 9.15207E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 30.39750 | 7.88225E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 35.46375 | 7.00597E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 40.53000 | 6.38014E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 45.59625 | 5.9133E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 50.66250 | 5.55104E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 3.03975 | 0.000728305 | 273.15 | 0.5048 | 0.4952 | Yes |
| 5.06625 | 0.000430348 | 273.15 | 0.5048 | 0.4952 | Yes |
| 7.59938 | 0.000282117 | 273.15 | 0.5048 | 0.4952 | Yes |
| 10.13250 | 0.000208652 | 273.15 | 0.5048 | 0.4952 | Yes |
| 12.66563 | 0.000165182 | 273.15 | 0.5048 | 0.4952 | Yes |
| 15.19875 | 0.00013668 | 273.15 | 0.5048 | 0.4952 | Yes |
| 17.73188 | 0.000116847 | 273.15 | 0.5048 | 0.4952 | Yes |
| 20.26500 | 0.000102465 | 273.15 | 0.5048 | 0.4952 | Yes |
| 22.79813 | 9.17279E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 25.33125 | 8.32993E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 30.39750 | 7.13437E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 35.46375 | 6.32714E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 40.53000 | 5.75311E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 45.59625 | 5.34747E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 50.66250 | 5.02611E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 3.03975 | 0.000741529 | 273.15 | 0.2513 | 0.7487 | Yes |
| 5.06625 | 0.000443572 | 273.15 | 0.2513 | 0.7487 | Yes |
| 7.59938 | 0.000295267 | 273.15 | 0.2513 | 0.7487 | Yes |
| 10.13250 | 0.000221652 | 273.15 | 0.2513 | 0.7487 | Yes |
| 12.66563 | 0.000177895 | 273.15 | 0.2513 | 0.7487 | Yes |
| 15.19875 | 0.000149053 | 273.15 | 0.2513 | 0.7487 | Yes |
| 17.73188 | 0.000128759 | 273.15 | 0.2513 | 0.7487 | Yes |
| 20.26500 | 0.000113807 | 273.15 | 0.2513 | 0.7487 | Yes |
| 22.79813 | 0.000102317 | 273.15 | 0.2513 | 0.7487 | Yes |
| 25.33125 | 9.33228E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 30.39750 | 8.00776E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 35.46375 | 7.09434E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 40.53000 | 6.43729E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 45.59625 | 5.9407E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 50.66250 | 5.54925E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 3.03975 | 0.000734207 | 273.15 | 0.5048 | 0.4952 | Yes |
| 5.06625 | 0.000435952 | 273.15 | 0.5048 | 0.4952 | Yes |
| 7.59938 | 0.000287347 | 273.15 | 0.5048 | 0.4952 | Yes |
| 10.13250 | 0.000213605 | 273.15 | 0.5048 | 0.4952 | Yes |
| 12.66563 | 0.000169898 | 273.15 | 0.5048 | 0.4952 | Yes |
| 15.19875 | 0.000141118 | 273.15 | 0.5048 | 0.4952 | Yes |
| 17.73188 | 0.000120959 | 273.15 | 0.5048 | 0.4952 | Yes |
| 20.26500 | 0.000106186 | 273.15 | 0.5048 | 0.4952 | Yes |
| 22.79813 | 9.50153E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 25.33125 | 8.624E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 30.39750 | 7.35776E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 35.46375 | 6.50005E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 40.53000 | 5.88591E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 45.59625 | 5.43862E-05 | 273.15 | 0.5048 | 0.4952 | Yes |
| 50.66250 | 5.07138E-05 | 273.15 | 0.5048 | 0.4952 | Yes |

Continued: Data summarised from TABLE II of Haney44 [108]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 3.03975 | 0.000744368 | 273.15 | 0.2513 | 0.7487 | Yes |
| 5.06625 | 0.000446352 | 273.15 | 0.2513 | 0.7487 | Yes |
| 7.59938 | 0.000297897 | 273.15 | 0.2513 | 0.7487 | Yes |
| 10.13250 | 0.00022414 | 273.15 | 0.2513 | 0.7487 | Yes |
| 12.66563 | 0.000180226 | 273.15 | 0.2513 | 0.7487 | Yes |
| 15.19875 | 0.000151205 | 273.15 | 0.2513 | 0.7487 | Yes |
| 17.73188 | 0.000130693 | 273.15 | 0.2513 | 0.7487 | Yes |
| 20.26500 | 0.00011551 | 273.15 | 0.2513 | 0.7487 | Yes |
| 22.79813 | 0.000103841 | 273.15 | 0.2513 | 0.7487 | Yes |
| 25.33125 | 9.46138E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 30.39750 | 8.10489E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 35.46375 | 7.16158E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 40.53000 | 6.53087E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 45.59625 | 5.95763E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 50.66250 | 5.54701E-05 | 273.15 | 0.2513 | 0.7487 | Yes |
| 4.69758 | 0.000430097 | 293.2 | 0.702400 | 0.297600 | Yes |
| 4.28804 | 0.000480128 | 293.2 | 0.702400 | 0.297600 | Yes |
| 4.00226 | 0.000521057 | 293.2 | 0.702400 | 0.297600 | Yes |
| 3.50269 | 0.000608533 | 293.2 | 0.702400 | 0.297600 | Yes |
| 3.00310 | 0.000724882 | 293.2 | 0.702400 | 0.297600 | Yes |
| 2.50368 | 0.000887384 | 293.2 | 0.702400 | 0.297600 | Yes |
| 2.00442 | 0.001130487 | 293.2 | 0.702400 | 0.297600 | Yes |
| 1.50699 | 0.001532498 | 293.2 | 0.702400 | 0.297600 | Yes |
| 1.00550 | 0.002339860 | 293.2 | 0.702400 | 0.297600 | Yes |
| 0.80569 | 0.002941322 | 293.2 | 0.702400 | 0.297600 | Yes |
| 0.60615 | 0.003937615 | 293.2 | 0.702400 | 0.297600 | Yes |
| 5.18106 | 0.000409518 | 293.2 | 0.539900 | 0.460100 | Yes |
| 4.18809 | 0.000520861 | 293.2 | 0.539900 | 0.460100 | Yes |
| 3.70248 | 0.000597156 | 293.2 | 0.539900 | 0.460100 | Yes |
| 3.20700 | 0.000698819 | 293.2 | 0.539900 | 0.460100 | Yes |
| 2.69969 | 0.000841641 | 293.2 | 0.539900 | 0.460100 | Yes |
| 2.20817 | 0.001042639 | 293.2 | 0.539900 | 0.460100 | Yes |
| 1.71058 | 0.001363788 | 293.2 | 0.539900 | 0.460100 | Yes |
| 1.44089 | 0.001630535 | 293.2 | 0.539900 | 0.460100 | Yes |
| 1.00646 | 0.002360839 | 293.2 | 0.539900 | 0.460100 | Yes |
| 0.80573 | 0.002964268 | 293.2 | 0.539900 | 0.460100 | Yes |
| 0.60297 | 0.003981678 | 293.2 | 0.539900 | 0.460100 | Yes |
| 4.05769 | 0.000549598 | 293.2 | 0.468600 | 0.531400 | Yes |
| 3.50024 | 0.000644900 | 293.2 | 0.468600 | 0.531400 | Yes |
| 3.00078 | 0.000760485 | 293.2 | 0.468600 | 0.531400 | Yes |
| 2.50151 | 0.000922334 | 293.2 | 0.468600 | 0.531400 | Yes |
| 2.00001 | 0.001166443 | 293.2 | 0.468600 | 0.531400 | Yes |
| 1.50165 | 0.001570698 | 293.2 | 0.468600 | 0.531400 | Yes |
| 1.00236 | 0.002379108 | 293.2 | 0.468600 | 0.531400 | Yes |
| 0.80172 | 0.002987644 | 293.2 | 0.468600 | 0.531400 | Yes |
| 0.60197 | 0.003996519 | 293.2 | 0.468600 | 0.531400 | Yes |

Data summarised from TABLE 1 of Jiang90 [107]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 4.53762 | 0.000510150 | 293.2 | 0.271200 | 0.728800 | Yes |
| 4.01826 | 0.000579211 | 293.2 | 0.271200 | 0.728800 | Yes |
| 3.51901 | 0.000664932 | 293.2 | 0.271200 | 0.728800 | Yes |
| 3.00972 | 0.000781806 | 293.2 | 0.271200 | 0.728800 | Yes |
| 2.50625 | 0.000944190 | 293.2 | 0.271200 | 0.728800 | Yes |
| 2.00715 | 0.001185738 | 293.2 | 0.271200 | 0.728800 | Yes |
| 1.51140 | 0.001583796 | 293.2 | 0.271200 | 0.728800 | Yes |
| 1.00979 | 0.002384688 | 293.2 | 0.271200 | 0.728800 | Yes |
| 0.80509 | 0.002998340 | 293.2 | 0.271200 | 0.728800 | Yes |
| 0.60840 | 0.003977091 | 293.2 | 0.271200 | 0.728800 | Yes |
| 5.950 | 0.000355641 | 313.05 | 0.6772 | 0.3228 | Yes |
| 8.825 | 0.000214003 | 313.05 | 0.6772 | 0.3228 | Yes |
| 10.863 | 0.000160437 | 313.05 | 0.6772 | 0.3228 | Yes |
| 17.698 | 0.000085872 | 313.05 | 0.6772 | 0.3228 | Yes |
| 20.619 | 0.000074995 | 313.05 | 0.6772 | 0.3228 | Yes |
| 23.548 | 0.000068275 | 313.05 | 0.6772 | 0.3228 | Yes |
| 26.480 | 0.000063762 | 313.05 | 0.6772 | 0.3228 | Yes |
| 29.414 | 0.000060437 | 313.05 | 0.6772 | 0.3228 | Yes |
| 32.350 | 0.000057937 | 313.05 | 0.6772 | 0.3228 | Yes |
| 35.287 | 0.000055940 | 313.05 | 0.6772 | 0.3228 | Yes |
| 38.224 | 0.000054304 | 313.05 | 0.6772 | 0.3228 | Yes |
| 41.162 | 0.000052894 | 313.05 | 0.6772 | 0.3228 | Yes |
| 44.101 | 0.000051694 | 313.05 | 0.6772 | 0.3228 | Yes |
| 47.037 | 0.000050665 | 313.05 | 0.6772 | 0.3228 | Yes |
| 49.978 | 0.000049756 | 313.05 | 0.6772 | 0.3228 | Yes |
| 52.917 | 0.000048940 | 313.05 | 0.6772 | 0.3228 | Yes |
| 55.858 | 0.000048181 | 313.05 | 0.6772 | 0.3228 | Yes |
| 58.795 | 0.000047509 | 313.05 | 0.6772 | 0.3228 | Yes |

Data summarised from TABLE 2 of Kosov75 [120]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 5.960 | 0.000391413 | 313.05 | 0.4706 | 0.5294 | Yes |
| 8.838 | 0.000251556 | 313.05 | 0.4706 | 0.5294 | Yes |
| 12.174 | 0.000174883 | 313.05 | 0.4706 | 0.5294 | Yes |
| 18.708 | 0.000110033 | 313.05 | 0.4706 | 0.5294 | Yes |
| 20.652 | 0.000100091 | 313.05 | 0.4706 | 0.5294 | Yes |
| 23.574 | 0.000089065 | 313.05 | 0.4706 | 0.5294 | Yes |
| 26.501 | 0.000081173 | 313.05 | 0.4706 | 0.5294 | Yes |
| 29.432 | 0.000075273 | 313.05 | 0.4706 | 0.5294 | Yes |
| 32.365 | 0.000070776 | 313.05 | 0.4706 | 0.5294 | Yes |
| 35.299 | 0.000067186 | 313.05 | 0.4706 | 0.5294 | Yes |
| 38.234 | 0.000064268 | 313.05 | 0.4706 | 0.5294 | Yes |
| 41.171 | 0.000061884 | 313.05 | 0.4706 | 0.5294 | Yes |
| 44.108 | 0.000059864 | 313.05 | 0.4706 | 0.5294 | Yes |
| 47.046 | 0.000058100 | 313.05 | 0.4706 | 0.5294 | Yes |
| 49.983 | 0.000056597 | 313.05 | 0.4706 | 0.5294 | Yes |
| 52.921 | 0.000055255 | 313.05 | 0.4706 | 0.5294 | Yes |
| 55.889 | 0.000054095 | 313.05 | 0.4706 | 0.5294 | Yes |
| 58.798 | 0.000053035 | 313.05 | 0.4706 | 0.5294 | Yes |
| 5.945 | 0.000420057 | 313.05 | 0.2329 | 0.7671 | Yes |
| 8.831 | 0.000279038 | 313.05 | 0.2329 | 0.7671 | Yes |
| 11.846 | 0.000206722 | 313.05 | 0.2329 | 0.7671 | Yes |
| 14.751 | 0.000166064 | 313.05 | 0.2329 | 0.7671 | Yes |
| 19.687 | 0.000126054 | 313.05 | 0.2329 | 0.7671 | Yes |
| 23.580 | 0.000107538 | 313.05 | 0.2329 | 0.7671 | Yes |
| 26.506 | 0.000097602 | 313.05 | 0.2329 | 0.7671 | Yes |
| 29.436 | 0.000089964 | 313.05 | 0.2329 | 0.7671 | Yes |
| 32.368 | 0.000083938 | 313.05 | 0.2329 | 0.7671 | Yes |
| 35.301 | 0.000079050 | 313.05 | 0.2329 | 0.7671 | Yes |
| 38.235 | 0.000075026 | 313.05 | 0.2329 | 0.7671 | Yes |
| 41.171 | 0.000071661 | 313.05 | 0.2329 | 0.7671 | Yes |
| 44.107 | 0.000068744 | 313.05 | 0.2329 | 0.7671 | Yes |
| 47.044 | 0.000066278 | 313.05 | 0.2329 | 0.7671 | Yes |
| 49.981 | 0.000064154 | 313.05 | 0.2329 | 0.7671 | Yes |
| 52.919 | 0.000062259 | 313.05 | 0.2329 | 0.7671 | Yes |
| 55.857 | 0.000060587 | 313.05 | 0.2329 | 0.7671 | Yes |
| 58.795 | 0.000059140 | 313.05 | 0.2329 | 0.7671 | Yes |
| 23.589 | 0.000091114 | 353.15 | 0.6772 | 0.3228 | Yes |
| 26.513 | 0.000082893 | 353.15 | 0.6772 | 0.3228 | Yes |
| 29.443 | 0.000076578 | 353.15 | 0.6772 | 0.3228 | Yes |
| 32.374 | 0.000071759 | 353.15 | 0.6772 | 0.3228 | Yes |
| 35.308 | 0.000067983 | 353.15 | 0.6772 | 0.3228 | Yes |
| 38.243 | 0.000064992 | 353.15 | 0.6772 | 0.3228 | Yes |
| 41.179 | 0.000062526 | 353.15 | 0.6772 | 0.3228 | Yes |
| 44.116 | 0.000060460 | 353.15 | 0.6772 | 0.3228 | Yes |
| 47.053 | 0.000058720 | 353.15 | 0.6772 | 0.3228 | Yes |
| 49.991 | 0.000057184 | 353.15 | 0.6772 | 0.3228 | Yes |
| 52.929 | 0.000055851 | 353.15 | 0.6772 | 0.3228 | Yes |
| 55.867 | 0.000054664 | 353.15 | 0.6772 | 0.3228 | Yes |
| 58.805 | 0.000053611 | 353.15 | 0.6772 | 0.3228 | Yes |
| 23.687 | 0.000110630 | 353.15 | 0.4706 | 0.5294 | Yes |
| 26.532 | 0.000100206 | 353.15 | 0.4706 | 0.5294 | Yes |
| 29.459 | 0.000091934 | 353.15 | 0.4706 | 0.5294 | Yes |
| 32.389 | 0.000085448 | 353.15 | 0.4706 | 0.5294 | Yes |
| 35.320 | 0.000080261 | 353.15 | 0.4706 | 0.5294 | Yes |
| 38.254 | 0.000076039 | 353.15 | 0.4706 | 0.5294 | Yes |
| 41.188 | 0.000072548 | 353.15 | 0.4706 | 0.5294 | Yes |
| 44.124 | 0.000069577 | 353.15 | 0.4706 | 0.5294 | Yes |
| 47.030 | 0.000067088 | 353.15 | 0.4706 | 0.5294 | Yes |
| 49.996 | 0.000064864 | 353.15 | 0.4706 | 0.5294 | Yes |
| 52.934 | 0.000062972 | 353.15 | 0.4706 | 0.5294 | Yes |
| 55.871 | 0.000061291 | 353.15 | 0.4706 | 0.5294 | Yes |
| 58.809 | 0.000059792 | 353.15 | 0.4706 | 0.5294 | Yes |
| 23.608 | 0.000126592 | 353.15 | 0.2329 | 0.7671 | Yes |
| 26.531 | 0.000114283 | 353.15 | 0.2329 | 0.7671 | Yes |
| 29.458 | 0.000105190 | 353.15 | 0.2329 | 0.7671 | Yes |
| 32.387 | 0.000097626 | 353.15 | 0.2329 | 0.7671 | Yes |
| 35.318 | 0.000091453 | 353.15 | 0.2329 | 0.7671 | Yes |
| 38.251 | 0.000086328 | 353.15 | 0.2329 | 0.7671 | Yes |
| 41.185 | 0.000082003 | 353.15 | 0.2329 | 0.7671 | Yes |
| 44.121 | 0.000078377 | 353.15 | 0.2329 | 0.7671 | Yes |
| 47.056 | 0.000075210 | 353.15 | 0.2329 | 0.7671 | Yes |
| 49.993 | 0.000072483 | 353.15 | 0.2329 | 0.7671 | Yes |
| 52.930 | 0.000070070 | 353.15 | 0.2329 | 0.7671 | Yes |
| 55.867 | 0.000067931 | 353.15 | 0.2329 | 0.7671 | Yes |
| 55.804 | 0.000069570 | 353.15 | 0.2329 | 0.7671 | Yes |

Continued: Data summarised from TABLE 2 of Kosov75 [120]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 5.06625 | 0.00046508 | 323.15 | 0.473 | 0.527 | Yes |
| 10.13250 | 0.00022219 | 323.15 | 0.473 | 0.527 | Yes |
| 20.26500 | 0.00011109 | 323.15 | 0.473 | 0.527 | Yes |
| 30.39750 | 0.00007994 | 323.15 | 0.473 | 0.527 | Yes |
| 40.53000 | 0.00006671 | 323.15 | 0.473 | 0.527 | Yes |
| 50.66250 | 0.00005914 | 323.15 | 0.473 | 0.527 | Yes |
| 5.06625 | 0.00055557 | 373.15 | 0.473 | 0.527 | Yes |
| 10.13250 | 0.00027779 | 373.15 | 0.473 | 0.527 | Yes |
| 20.26500 | 0.00013829 | 373.15 | 0.473 | 0.527 | Yes |
| 30.39750 | 0.00009770 | 373.15 | 0.473 | 0.527 | Yes |
| 40.53000 | 0.00007962 | 373.15 | 0.473 | 0.527 | Yes |
| 50.66250 | 0.00006916 | 373.15 | 0.473 | 0.527 | Yes |
| 5.06625 | 0.00063787 | 423.15 | 0.473 | 0.527 | Yes |
| 10.13250 | 0.00033328 | 423.15 | 0.473 | 0.527 | Yes |
| 20.26500 | 0.00016889 | 423.15 | 0.473 | 0.527 | Yes |
| 30.39750 | 0.00011639 | 423.15 | 0.473 | 0.527 | Yes |
| 40.53000 | 0.00009302 | 423.15 | 0.473 | 0.527 | Yes |
| 50.66250 | 0.00007955 | 423.15 | 0.473 | 0.527 | Yes |
| 5.06625 | 0.00074626 | 473.15 | 0.473 | 0.527 | Yes |
| 10.13250 | 0.00037878 | 473.15 | 0.473 | 0.527 | Yes |
| 20.26500 | 0.00019489 | 473.15 | 0.473 | 0.527 | Yes |
| 30.39750 | 0.00013589 | 473.15 | 0.473 | 0.527 | Yes |
| 40.53000 | 0.00010809 | 473.15 | 0.473 | 0.527 | Yes |
| 50.66250 | 0.00009200 | 473.15 | 0.473 | 0.527 | Yes |
| 5.06625 | 0.00038757 | 273.15 | 0.242 | 0.758 | Yes |
| 10.13250 | 0.00019208 | 273.15 | 0.242 | 0.758 | Yes |
| 20.26500 | 0.00009666 | 273.15 | 0.242 | 0.758 | Yes |
| 30.39750 | 0.00007183 | 273.15 | 0.242 | 0.758 | Yes |
| 40.53000 | 0.00006135 | 273.15 | 0.242 | 0.758 | Yes |
| 50.66250 | 0.00005507 | 273.15 | 0.242 | 0.758 | Yes |
| 5.06625 | 0.00050246 | 323.15 | 0.242 | 0.758 | Yes |
| 10.13250 | 0.00024838 | 323.15 | 0.242 | 0.758 | Yes |
| 20.26500 | 0.00012719 | 323.15 | 0.242 | 0.758 | Yes |
| 30.39750 | 0.00009061 | 323.15 | 0.242 | 0.758 | Yes |
| 40.53000 | 0.00007428 | 323.15 | 0.242 | 0.758 | Yes |
| 50.66250 | 0.00006514 | 323.15 | 0.242 | 0.758 | Yes |
| 5.06625 | 0.00058815 | 373.15 | 0.242 | 0.758 | Yes |
| 10.13250 | 0.00029938 | 373.15 | 0.242 | 0.758 | Yes |
| 20.26500 | 0.00015309 | 373.15 | 0.242 | 0.758 | Yes |
| 30.39750 | 0.00010889 | 373.15 | 0.242 | 0.758 | Yes |
| 40.53000 | 0.00008759 | 373.15 | 0.242 | 0.758 | Yes |
| 50.66250 | 0.00007512 | 373.15 | 0.242 | 0.758 | Yes |
| 5.06625 | 0.00068484 | 423.15 | 0.242 | 0.758 | Yes |
| 10.13250 | 0.00034717 | 423.15 | 0.242 | 0.758 | Yes |
| 20.26500 | 0.00017919 | 423.15 | 0.242 | 0.758 | Yes |
| 30.39750 | 0.00012529 | 423.15 | 0.242 | 0.758 | Yes |
| 40.53000 | 0.00009999 | 423.15 | 0.242 | 0.758 | Yes |
| 50.66250 | 0.00008524 | 423.15 | 0.242 | 0.758 | Yes |
| 5.06625 | 0.00076334 | 473.15 | 0.242 | 0.758 | Yes |
| 10.13250 | 0.00038607 | 473.15 | 0.242 | 0.758 | Yes |
| 20.26500 | 0.00020258 | 473.15 | 0.242 | 0.758 | Yes |
| 30.39750 | 0.00014269 | 473.15 | 0.242 | 0.758 | Yes |
| 40.53000 | 0.00011349 | 473.15 | 0.242 | 0.758 | Yes |
| 50.66250 | 0.00009582 | 473.15 | 0.242 | 0.758 | Yes |

Data summarised from Table 1 of Kritschewsky40 [99]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 1.001 | 0.002420212 | 303.22 | 0.9585 | 0.0415 | Yes |
| 2.000 | 0.001148238 | 303.22 | 0.9585 | 0.0415 | Yes |
| 3.001 | 0.000720991 | 303.22 | 0.9585 | 0.0415 | Yes |
| 4.001 | 0.000506083 | 303.22 | 0.9585 | 0.0415 | Yes |
| 5.001 | 0.000372452 | 303.22 | 0.9585 | 0.0415 | Yes |
| 6.000 | 0.000277912 | 303.22 | 0.9585 | 0.0415 | Yes |
| 7.001 | 0.000203226 | 303.22 | 0.9585 | 0.0415 | Yes |
| 8.001 | 0.000130986 | 303.22 | 0.9585 | 0.0415 | Yes |
| 9.001 | 7.96011E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 10.002 | 6.82915E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 11.001 | 6.34539E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 12.001 | 6.0567E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 13.001 | 5.8548E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 14.002 | 5.70853E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 15.004 | 5.59527E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 16.001 | 5.49637E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 17.003 | 5.4077E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 18.001 | 5.32827E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 19.005 | 5.25776E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 20.001 | 5.19998E-05 | 303.22 | 0.9585 | 0.0415 | Yes |
| 1.001 | 0.002581656 | 323.18 | 0.9585 | 0.0415 | Yes |
| 2.004 | 0.001240229 | 323.18 | 0.9585 | 0.0415 | Yes |
| 3.000 | 0.000792142 | 323.18 | 0.9585 | 0.0415 | Yes |
| 4.001 | 0.000566985 | 323.18 | 0.9585 | 0.0415 | Yes |
| 5.003 | 0.00043002 | 323.18 | 0.9585 | 0.0415 | Yes |
| 6.001 | 0.000337323 | 323.18 | 0.9585 | 0.0415 | Yes |
| 7.001 | 0.000269247 | 323.18 | 0.9585 | 0.0415 | Yes |
| 8.001 | 0.000216287 | 323.18 | 0.9585 | 0.0415 | Yes |
| 9.001 | 0.000173571 | 323.18 | 0.9585 | 0.0415 | Yes |
| 10.001 | 0.00013857 | 323.18 | 0.9585 | 0.0415 | Yes |
| 11.002 | 0.000111249 | 323.18 | 0.9585 | 0.0415 | Yes |
| 12.001 | 9.27524E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 13.001 | 8.14376E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 14.001 | 7.43767E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 15.002 | 6.99298E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 16.001 | 6.67437E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 17.001 | 6.43717E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 18.003 | 6.24861E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 19.002 | 6.08938E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 20.001 | 5.95281E-05 | 323.18 | 0.9585 | 0.0415 | Yes |
| 1.003 | 0.002851711 | 343.15 | 0.9585 | 0.0415 | Yes |
| 2.001 | 0.001344896 | 343.15 | 0.9585 | 0.0415 | Yes |
| 3.001 | 0.000864844 | 343.15 | 0.9585 | 0.0415 | Yes |
| 4.002 | 0.000632604 | 343.15 | 0.9585 | 0.0415 | Yes |
| 5.003 | 0.000485235 | 343.15 | 0.9585 | 0.0415 | Yes |
| 6.002 | 0.000387052 | 343.15 | 0.9585 | 0.0415 | Yes |
| 7.000 | 0.000317414 | 343.15 | 0.9585 | 0.0415 | Yes |
| 8.001 | 0.000264773 | 343.15 | 0.9585 | 0.0415 | Yes |
| 9.000 | 0.000223721 | 343.15 | 0.9585 | 0.0415 | Yes |

Data summarised from Table 4 and 5 of Mantovani12 [109]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 10.001 | 0.000190758 | 343.15 | 0.9585 | 0.0415 | Yes |
| 11.002 | 0.000163891 | 343.15 | 0.9585 | 0.0415 | Yes |
| 12.000 | 0.000142002 | 343.15 | 0.9585 | 0.0415 | Yes |
| 13.000 | 0.00012429 | 343.15 | 0.9585 | 0.0415 | Yes |
| 14.000 | 0.000110295 | 343.15 | 0.9585 | 0.0415 | Yes |
| 15.001 | 9.94288E-05 | 343.15 | 0.9585 | 0.0415 | Yes |
| 16.001 | 9.11185E-05 | 343.15 | 0.9585 | 0.0415 | Yes |
| 17.003 | 8.48375E-05 | 343.15 | 0.9585 | 0.0415 | Yes |
| 18.001 | 7.9986E-05 | 343.15 | 0.9585 | 0.0415 | Yes |
| 19.002 | 7.61231E-05 | 343.15 | 0.9585 | 0.0415 | Yes |
| 20.004 | 7.30075E-05 | 343.15 | 0.9585 | 0.0415 | Yes |
| 1.002 | 0.003089522 | 363.15 | 0.9585 | 0.0415 | Yes |
| 2.002 | 0.001426324 | 363.15 | 0.9585 | 0.0415 | Yes |
| 3.000 | 0.000930771 | 363.15 | 0.9585 | 0.0415 | Yes |
| 4.002 | 0.000680151 | 363.15 | 0.9585 | 0.0415 | Yes |
| 5.001 | 0.000529708 | 363.15 | 0.9585 | 0.0415 | Yes |
| 6.001 | 0.00042832 | 363.15 | 0.9585 | 0.0415 | Yes |
| 7.002 | 0.000356464 | 363.15 | 0.9585 | 0.0415 | Yes |
| 8.005 | 0.000302105 | 363.15 | 0.9585 | 0.0415 | Yes |
| 9.003 | 0.000260118 | 363.15 | 0.9585 | 0.0415 | Yes |
| 10.001 | 0.000226492 | 363.15 | 0.9585 | 0.0415 | Yes |
| 11.002 | 0.00019899 | 363.15 | 0.9585 | 0.0415 | Yes |
| 12.002 | 0.000176304 | 363.15 | 0.9585 | 0.0415 | Yes |
| 13.001 | 0.000157582 | 363.15 | 0.9585 | 0.0415 | Yes |
| 14.000 | 0.000141881 | 363.15 | 0.9585 | 0.0415 | Yes |
| 15.001 | 0.000128795 | 363.15 | 0.9585 | 0.0415 | Yes |
| 16.002 | 0.000117907 | 363.15 | 0.9585 | 0.0415 | Yes |
| 17.001 | 0.000108959 | 363.15 | 0.9585 | 0.0415 | Yes |
| 18.001 | 0.000101527 | 363.15 | 0.9585 | 0.0415 | Yes |
| 19.001 | 9.5354E-05 | 363.15 | 0.9585 | 0.0415 | Yes |
| 20.002 | 9.01445E-05 | 363.15 | 0.9585 | 0.0415 | Yes |
| 1.002 | 0.003313914 | 383.14 | 0.9585 | 0.0415 | Yes |
| 2.001 | 0.001573358 | 383.14 | 0.9585 | 0.0415 | Yes |
| 3.000 | 0.001013942 | 383.14 | 0.9585 | 0.0415 | Yes |
| 4.003 | 0.000739693 | 383.14 | 0.9585 | 0.0415 | Yes |
| 5.003 | 0.000578332 | 383.14 | 0.9585 | 0.0415 | Yes |
| 6.000 | 0.000470641 | 383.14 | 0.9585 | 0.0415 | Yes |
| 7.003 | 0.00039427 | 383.14 | 0.9585 | 0.0415 | Yes |
| 8.001 | 0.000337087 | 383.14 | 0.9585 | 0.0415 | Yes |
| 9.002 | 0.000292562 | 383.14 | 0.9585 | 0.0415 | Yes |
| 10.001 | 0.000257216 | 383.14 | 0.9585 | 0.0415 | Yes |
| 11.002 | 0.000228197 | 383.14 | 0.9585 | 0.0415 | Yes |
| 12.002 | 0.000204347 | 383.14 | 0.9585 | 0.0415 | Yes |
| 13.002 | 0.000184585 | 383.14 | 0.9585 | 0.0415 | Yes |
| 14.002 | 0.000167767 | 383.14 | 0.9585 | 0.0415 | Yes |
| 15.002 | 0.000153524 | 383.14 | 0.9585 | 0.0415 | Yes |
| 16.001 | 0.000141349 | 383.14 | 0.9585 | 0.0415 | Yes |
| 17.001 | 0.000130947 | 383.14 | 0.9585 | 0.0415 | Yes |
| 1.000 | 0.002436487 | 303.22 | 0.9021 | 0.0979 | Yes |
| 2.000 | 0.001159028 | 303.22 | 0.9021 | 0.0979 | Yes |
| 3.001 | 0.000731282 | 303.22 | 0.9021 | 0.0979 | Yes |
| 4.001 | 0.000516849 | 303.22 | 0.9021 | 0.0979 | Yes |
| 5.000 | 0.00038543 | 303.22 | 0.9021 | 0.0979 | Yes |
| 6.002 | 0.000294747 | 303.22 | 0.9021 | 0.0979 | Yes |
| 7.000 | 0.000226789 | 303.22 | 0.9021 | 0.0979 | Yes |
| 8.001 | 0.000170621 | 303.22 | 0.9021 | 0.0979 | Yes |
| 9.000 | 0.000124126 | 303.22 | 0.9021 | 0.0979 | Yes |
| 10.003 | 9.35046E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 11.002 | 7.84076E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 12.003 | 7.08078E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 13.000 | 6.62922E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 14.002 | 6.32137E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 15.002 | 6.10655E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 16.001 | 5.93584E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 17.005 | 5.79846E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 18.001 | 5.67542E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 19.003 | 5.57185E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 20.001 | 5.48757E-05 | 303.22 | 0.9021 | 0.0979 | Yes |
| 1.002 | 0.002628087 | 323.18 | 0.9021 | 0.0979 | Yes |
| 2.000 | 0.001264331 | 323.18 | 0.9021 | 0.0979 | Yes |
| 3.003 | 0.000805687 | 323.18 | 0.9021 | 0.0979 | Yes |
| 4.001 | 0.000578882 | 323.18 | 0.9021 | 0.0979 | Yes |
| 5.001 | 0.000442813 | 323.18 | 0.9021 | 0.0979 | Yes |
| 6.000 | 0.000350658 | 323.18 | 0.9021 | 0.0979 | Yes |
| 7.002 | 0.000283543 | 323.18 | 0.9021 | 0.0979 | Yes |
| 8.001 | 0.000232682 | 323.18 | 0.9021 | 0.0979 | Yes |
| 9.000 | 0.000192322 | 323.18 | 0.9021 | 0.0979 | Yes |
| 10.001 | 0.000159911 | 323.18 | 0.9021 | 0.0979 | Yes |
| 11.002 | 0.000134175 | 323.18 | 0.9021 | 0.0979 | Yes |
| 12.001 | 0.000114169 | 323.18 | 0.9021 | 0.0979 | Yes |
| 13.000 | 9.96048E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 14.002 | 8.91728E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 15.001 | 8.17559E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 16.000 | 7.65425E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 17.001 | 7.26413E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 18.000 | 6.95763E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 19.001 | 6.70738E-05 | 323.18 | 0.9021 | 0.0979 | Yes |
| 20.001 | 6.50008E-05 | 323.18 | 0.9021 | 0.0979 | Yes |

Continued: Data summarised from Table 4 and 5 of Mantovani12 [109]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 1.001 | 0.002970161 | 343.15 | 0.9021 | 0.0979 | Yes |
| 2.003 | 0.001383429 | 343.15 | 0.9021 | 0.0979 | Yes |
| 3.001 | 0.000892422 | 343.15 | 0.9021 | 0.0979 | Yes |
| 4.001 | 0.000641821 | 343.15 | 0.9021 | 0.0979 | Yes |
| 5.003 | 0.000493702 | 343.15 | 0.9021 | 0.0979 | Yes |
| 6.003 | 0.000396188 | 343.15 | 0.9021 | 0.0979 | Yes |
| 7.003 | 0.00032659 | 343.15 | 0.9021 | 0.0979 | Yes |
| 8.001 | 0.00027484 | 343.15 | 0.9021 | 0.0979 | Yes |
| 9.002 | 0.000234236 | 343.15 | 0.9021 | 0.0979 | Yes |
| 10.000 | 0.000201987 | 343.15 | 0.9021 | 0.0979 | Yes |
| 11.001 | 0.000175721 | 343.15 | 0.9021 | 0.0979 | Yes |
| 12.002 | 0.000154206 | 343.15 | 0.9021 | 0.0979 | Yes |
| 13.001 | 0.000136668 | 343.15 | 0.9021 | 0.0979 | Yes |
| 14.001 | 0.000122397 | 343.15 | 0.9021 | 0.0979 | Yes |
| 15.001 | 0.000110894 | 343.15 | 0.9021 | 0.0979 | Yes |
| 16.000 | 0.00010163 | 343.15 | 0.9021 | 0.0979 | Yes |
| 17.002 | 9.43044E-05 | 343.15 | 0.9021 | 0.0979 | Yes |
| 18.002 | 8.84113E-05 | 343.15 | 0.9021 | 0.0979 | Yes |
| 19.001 | 8.35965E-05 | 343.15 | 0.9021 | 0.0979 | Yes |
| 20.002 | 7.96719E-05 | 343.15 | 0.9021 | 0.0979 | Yes |
| 1.001 | 0.003160357 | 363.15 | 0.9021 | 0.0979 | Yes |
| 2.001 | 0.0014856 | 363.15 | 0.9021 | 0.0979 | Yes |
| 3.000 | 0.000958528 | 363.15 | 0.9021 | 0.0979 | Yes |
| 4.003 | 0.000686013 | 363.15 | 0.9021 | 0.0979 | Yes |
| 5.003 | 0.00053631 | 363.15 | 0.9021 | 0.0979 | Yes |
| 6.001 | 0.000435051 | 363.15 | 0.9021 | 0.0979 | Yes |
| 7.001 | 0.000363045 | 363.15 | 0.9021 | 0.0979 | Yes |
| 8.004 | 0.000309423 | 363.15 | 0.9021 | 0.0979 | Yes |
| 9.002 | 0.000267732 | 363.15 | 0.9021 | 0.0979 | Yes |
| 10.001 | 0.000234301 | 363.15 | 0.9021 | 0.0979 | Yes |
| 11.001 | 0.000207173 | 363.15 | 0.9021 | 0.0979 | Yes |
| 12.000 | 0.000184794 | 363.15 | 0.9021 | 0.0979 | Yes |
| 13.002 | 0.0001661 | 363.15 | 0.9021 | 0.0979 | Yes |
| 14.000 | 0.000150488 | 363.15 | 0.9021 | 0.0979 | Yes |
| 15.001 | 0.000137358 | 363.15 | 0.9021 | 0.0979 | Yes |
| 16.001 | 0.000126309 | 363.15 | 0.9021 | 0.0979 | Yes |
| 17.003 | 0.000117002 | 363.15 | 0.9021 | 0.0979 | Yes |
| 18.000 | 0.000109199 | 363.15 | 0.9021 | 0.0979 | Yes |
| 19.001 | 0.000102622 | 363.15 | 0.9021 | 0.0979 | Yes |
| 20.001 | 9.68988E-05 | 363.15 | 0.9021 | 0.0979 | Yes |
| 1.000 | 0.003400929 | 383.14 | 0.9021 | 0.0979 | Yes |
| 2.003 | 0.00159084 | 383.14 | 0.9021 | 0.0979 | Yes |
| 3.001 | 0.001022737 | 383.14 | 0.9021 | 0.0979 | Yes |
| 4.001 | 0.000746064 | 383.14 | 0.9021 | 0.0979 | Yes |
| 5.002 | 0.000584542 | 383.14 | 0.9021 | 0.0979 | Yes |
| 6.001 | 0.000477055 | 383.14 | 0.9021 | 0.0979 | Yes |
| 7.000 | 0.000400411 | 383.14 | 0.9021 | 0.0979 | Yes |
| 8.003 | 0.000343145 | 383.14 | 0.9021 | 0.0979 | Yes |
| 9.001 | 0.000298835 | 383.14 | 0.9021 | 0.0979 | Yes |
| 10.000 | 0.00026333 | 383.14 | 0.9021 | 0.0979 | Yes |
| 11.001 | 0.000234625 | 383.14 | 0.9021 | 0.0979 | Yes |
| 12.002 | 0.000210942 | 383.14 | 0.9021 | 0.0979 | Yes |
| 13.000 | 0.000191179 | 383.14 | 0.9021 | 0.0979 | Yes |
| 14.002 | 0.000174414 | 383.14 | 0.9021 | 0.0979 | Yes |
| 15.001 | 0.000160189 | 383.14 | 0.9021 | 0.0979 | Yes |
| 16.001 | 0.000148026 | 383.14 | 0.9021 | 0.0979 | Yes |
| 17.001 | 0.00013746 | 383.14 | 0.9021 | 0.0979 | Yes |
| 18.001 | 0.000128318 | 383.14 | 0.9021 | 0.0979 | Yes |
| 19.002 | 0.000120524 | 383.14 | 0.9021 | 0.0979 | Yes |
| 20.002 | 0.000113775 | 383.14 | 0.9021 | 0.0979 | Yes |

Continued: Data summarised from Table 4 and 5 of Mantovani12 [109]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 19.86622 | 9.78254E-05 | 250.044 | 0.10 | 0.90 | Yes |
| 18.04077 | 0.000106271 | 250.044 | 0.10 | 0.90 | Yes |
| 16.02422 | 0.000118332 | 250.044 | 0.10 | 0.90 | Yes |
| 14.01532 | 0.000134471 | 250.044 | 0.10 | 0.90 | Yes |
| 12.01104 | 0.000156813 | 250.045 | 0.10 | 0.90 | Yes |
| 10.00715 | 0.000189166 | 250.046 | 0.10 | 0.90 | Yes |
| 8.00002 | 0.000239157 | 250.047 | 0.10 | 0.90 | Yes |
| 5.99883 | 0.000323925 | 250.048 | 0.10 | 0.90 | Yes |
| 3.99732 | 0.000495706 | 250.047 | 0.10 | 0.90 | Yes |
| 1.98511 | 0.001021034 | 250.046 | 0.10 | 0.90 | Yes |
| 19.84087 | 0.000112825 | 275.019 | 0.10 | 0.90 | Yes |
| 18.05655 | 0.000122635 | 275.019 | 0.10 | 0.90 | Yes |
| 16.02186 | 0.000136874 | 275.018 | 0.10 | 0.90 | Yes |
| 14.01343 | 0.000155488 | 275.016 | 0.10 | 0.90 | Yes |
| 12.00866 | 0.000180904 | 275.017 | 0.10 | 0.90 | Yes |
| 10.00450 | 0.000217257 | 275.016 | 0.10 | 0.90 | Yes |
| 7.99787 | 0.000272891 | 275.012 | 0.10 | 0.90 | Yes |
| 6.00199 | 0.000366347 | 275.009 | 0.10 | 0.90 | Yes |
| 3.99710 | 0.000555785 | 275.019 | 0.10 | 0.90 | Yes |

Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 19.16513 | 0.000130961 | 299.963 | 0.10 | 0.90 | Yes |
| 17.86924 | 0.000139509 | 299.966 | 0.10 | 0.90 | Yes |
| 16.01378 | 0.000154356 | 299.967 | 0.10 | 0.90 | Yes |
| 14.00977 | 0.000175181 | 299.966 | 0.10 | 0.90 | Yes |
| 12.00591 | 0.000203435 | 299.966 | 0.10 | 0.90 | Yes |
| 10.00204 | 0.000243597 | 299.967 | 0.10 | 0.90 | Yes |
| 7.99970 | 0.000304586 | 299.967 | 0.10 | 0.90 | Yes |
| 5.99638 | 0.000407335 | 299.967 | 0.10 | 0.90 | Yes |
| 3.99646 | 0.000614061 | 299.968 | 0.10 | 0.90 | Yes |
| 1.99790 | 0.001236584 | 299.967 | 0.10 | 0.90 | Yes |
| 19.62110 | 0.00014211 | 324.979 | 0.10 | 0.90 | Yes |
| 18.00085 | 0.000153587 | 324.980 | 0.10 | 0.90 | Yes |
| 16.00130 | 0.000171185 | 324.979 | 0.10 | 0.90 | Yes |
| 13.98251 | 0.000194374 | 324.979 | 0.10 | 0.90 | Yes |
| 11.99919 | 0.000225128 | 324.979 | 0.10 | 0.90 | Yes |
| 9.99890 | 0.000268969 | 324.978 | 0.10 | 0.90 | Yes |
| 8.01923 | 0.000334497 | 324.978 | 0.10 | 0.90 | Yes |
| 5.99183 | 0.000447274 | 324.978 | 0.10 | 0.90 | Yes |
| 3.99616 | 0.000671261 | 324.978 | 0.10 | 0.90 | Yes |
| 1.99599 | 0.001347195 | 324.980 | 0.10 | 0.90 | Yes |
| 19.37788 | 0.000157217 | 349.967 | 0.10 | 0.90 | Yes |
| 17.99350 | 0.000168117 | 349.967 | 0.10 | 0.90 | Yes |
| 15.99987 | 0.000187305 | 349.966 | 0.10 | 0.90 | Yes |
| 13.99498 | 0.000212372 | 349.966 | 0.10 | 0.90 | Yes |
| 11.99755 | 0.000245985 | 349.966 | 0.10 | 0.90 | Yes |
| 9.99755 | 0.000293482 | 349.966 | 0.10 | 0.90 | Yes |
| 7.99575 | 0.000365326 | 349.966 | 0.10 | 0.90 | Yes |
| 5.99670 | 0.000485585 | 349.965 | 0.10 | 0.90 | Yes |
| 3.99656 | 0.000727358 | 349.964 | 0.10 | 0.90 | Yes |
| 1.99606 | 0.001455752 | 349.964 | 0.10 | 0.90 | Yes |
| 18.71878 | 0.000175779 | 374.975 | 0.10 | 0.90 | Yes |
| 17.96004 | 0.000182511 | 374.975 | 0.10 | 0.90 | Yes |
| 15.96599 | 0.000203384 | 374.974 | 0.10 | 0.90 | Yes |
| 13.97204 | 0.000230421 | 374.974 | 0.10 | 0.90 | Yes |
| 11.98120 | 0.000266651 | 374.974 | 0.10 | 0.90 | Yes |
| 9.98248 | 0.000317881 | 374.973 | 0.10 | 0.90 | Yes |
| 7.98995 | 0.00039489 | 374.973 | 0.10 | 0.90 | Yes |
| 5.99454 | 0.000523904 | 374.973 | 0.10 | 0.90 | Yes |
| 3.96223 | 0.000789726 | 374.970 | 0.10 | 0.90 | Yes |
| 1.97464 | 0.001580633 | 374.969 | 0.10 | 0.90 | Yes |
| 18.90806 | 0.000187244 | 400.038 | 0.10 | 0.90 | Yes |
| 17.81457 | 0.000197669 | 400.037 | 0.10 | 0.90 | Yes |
| 15.98414 | 0.000218408 | 400.035 | 0.10 | 0.90 | Yes |
| 13.99217 | 0.000247317 | 400.036 | 0.10 | 0.90 | Yes |
| 11.98674 | 0.000286355 | 400.035 | 0.10 | 0.90 | Yes |
| 9.99291 | 0.000340956 | 400.034 | 0.10 | 0.90 | Yes |
| 7.98095 | 0.000424103 | 400.035 | 0.10 | 0.90 | Yes |
| 5.99205 | 0.000561646 | 400.036 | 0.10 | 0.90 | Yes |
| 3.99487 | 0.000838311 | 400.034 | 0.10 | 0.90 | Yes |
| 1.99589 | 0.001670805 | 400.037 | 0.10 | 0.90 | Yes |
| 19.99666 | 9.32179E-05 | 250.059 | 0.15 | 0.85 | Yes |
| 18.01935 | 0.000101924 | 250.063 | 0.15 | 0.85 | Yes |
| 16.01636 | 0.000113523 | 250.064 | 0.15 | 0.85 | Yes |
| 14.01375 | 0.000129235 | 250.066 | 0.15 | 0.85 | Yes |
| 12.00577 | 0.000151284 | 250.066 | 0.15 | 0.85 | Yes |
| 10.00316 | 0.000183374 | 250.066 | 0.15 | 0.85 | Yes |
| 7.99621 | 0.000233229 | 250.064 | 0.15 | 0.85 | Yes |
| 5.98407 | 0.000318626 | 250.064 | 0.15 | 0.85 | Yes |
| 3.98271 | 0.000491443 | 250.061 | 0.15 | 0.85 | Yes |
| 1.94406 | 0.001036575 | 250.061 | 0.15 | 0.85 | Yes |
| 19.98318 | 0.000108524 | 275.028 | 0.15 | 0.85 | Yes |
| 17.99374 | 0.000119165 | 275.027 | 0.15 | 0.85 | Yes |
| 15.98143 | 0.00013309 | 275.027 | 0.15 | 0.85 | Yes |
| 14.00115 | 0.000151278 | 275.026 | 0.15 | 0.85 | Yes |
| 12.00000 | 0.000176479 | 275.026 | 0.15 | 0.85 | Yes |
| 9.99554 | 0.000212729 | 275.026 | 0.15 | 0.85 | Yes |
| 7.99430 | 0.000268154 | 275.025 | 0.15 | 0.85 | Yes |
| 5.99802 | 0.000361645 | 275.022 | 0.15 | 0.85 | Yes |
| 4.00063 | 0.000550357 | 275.019 | 0.15 | 0.85 | Yes |
| 1.98846 | 0.00112663 | 275.019 | 0.15 | 0.85 | Yes |
| 19.97735 | 0.000123058 | 299.963 | 0.15 | 0.85 | Yes |
| 17.99426 | 0.000135285 | 299.965 | 0.15 | 0.85 | Yes |
| 15.96936 | 0.000151242 | 299.968 | 0.15 | 0.85 | Yes |
| 13.99130 | 0.000171721 | 299.967 | 0.15 | 0.85 | Yes |
| 12.00779 | 0.000199568 | 299.968 | 0.15 | 0.85 | Yes |
| 10.00322 | 0.000239598 | 299.966 | 0.15 | 0.85 | Yes |
| 8.00779 | 0.000300197 | 299.966 | 0.15 | 0.85 | Yes |
| 5.99919 | 0.000402958 | 299.966 | 0.15 | 0.85 | Yes |
| 3.98234 | 0.00061197 | 299.967 | 0.15 | 0.85 | Yes |
| 1.99212 | 0.001235426 | 299.969 | 0.15 | 0.85 | Yes |
| 19.97825 | 0.000137045 | 324.980 | 0.15 | 0.85 | Yes |
| 18.01598 | 0.000150539 | 324.980 | 0.15 | 0.85 | Yes |
| 16.00631 | 0.000168073 | 324.981 | 0.15 | 0.85 | Yes |
| 14.01385 | 0.000190772 | 324.981 | 0.15 | 0.85 | Yes |
| 11.99115 | 0.000221968 | 324.981 | 0.15 | 0.85 | Yes |
| 9.99694 | 0.000265601 | 324.981 | 0.15 | 0.85 | Yes |
| 19.98296 | 0.000150419 | 349.967 | 0.15 | 0.85 | Yes |

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 18.00779 | 0.00016536 | 349.967 | 0.15 | 0.85 | Yes |
| 16.00783 | 0.00018448 | 349.967 | 0.15 | 0.85 | Yes |
| 14.00355 | 0.000209405 | 349.967 | 0.15 | 0.85 | Yes |
| 11.99797 | 0.000243033 | 349.967 | 0.15 | 0.85 | Yes |
| 9.99946 | 0.000290382 | 349.967 | 0.15 | 0.85 | Yes |
| 7.99535 | 0.000362201 | 349.967 | 0.15 | 0.85 | Yes |
| 5.99688 | 0.000482323 | 349.967 | 0.15 | 0.85 | Yes |
| 3.99534 | 0.000724168 | 349.967 | 0.15 | 0.85 | Yes |
| 1.99594 | 0.001451759 | 349.967 | 0.15 | 0.85 | Yes |
| 19.97235 | 0.00016352 | 374.956 | 0.15 | 0.85 | Yes |
| 17.99229 | 0.000179833 | 374.956 | 0.15 | 0.85 | Yes |
| 15.99852 | 0.000200533 | 374.956 | 0.15 | 0.85 | Yes |
| 13.98957 | 0.000227594 | 374.956 | 0.15 | 0.85 | Yes |
| 11.94535 | 0.000264776 | 374.955 | 0.15 | 0.85 | Yes |
| 9.98626 | 0.000315041 | 374.954 | 0.15 | 0.85 | Yes |
| 7.99726 | 0.000391745 | 374.954 | 0.15 | 0.85 | Yes |
| 5.99557 | 0.000520915 | 374.954 | 0.15 | 0.85 | Yes |
| 3.95365 | 0.000788416 | 374.953 | 0.15 | 0.85 | Yes |
| 1.96362 | 0.001586167 | 374.955 | 0.15 | 0.85 | Yes |
| 17.81821 | 0.000195515 | 400.023 | 0.15 | 0.85 | Yes |
| 15.97720 | 0.000216313 | 400.022 | 0.15 | 0.85 | Yes |
| 13.98802 | 0.000245135 | 400.022 | 0.15 | 0.85 | Yes |
| 11.98638 | 0.000284033 | 400.020 | 0.15 | 0.85 | Yes |
| 9.99083 | 0.000338626 | 400.020 | 0.15 | 0.85 | Yes |
| 7.99123 | 0.00042108 | 400.021 | 0.15 | 0.85 | Yes |
| 5.99535 | 0.000558761 | 400.019 | 0.15 | 0.85 | Yes |
| 3.99567 | 0.000835508 | 400.020 | 0.15 | 0.85 | Yes |
| 1.99535 | 0.00166877 | 400.019 | 0.15 | 0.85 | Yes |
| 19.63290 | 9.02991E-05 | 250.020 | 0.20 | 0.80 | Yes |
| 18.03870 | 9.70916E-05 | 250.020 | 0.20 | 0.80 | Yes |
| 17.63930 | 9.90853E-05 | 250.047 | 0.20 | 0.80 | Yes |
| 17.01160 | 0.000102396 | 250.046 | 0.20 | 0.80 | Yes |
| 16.02670 | 0.000108223 | 250.019 | 0.20 | 0.80 | Yes |
| 15.00850 | 0.000115374 | 250.047 | 0.20 | 0.80 | Yes |
| 14.01750 | 0.000123486 | 250.020 | 0.20 | 0.80 | Yes |
| 13.00490 | 0.000133454 | 250.046 | 0.20 | 0.80 | Yes |
| 12.01020 | 0.000145095 | 250.020 | 0.20 | 0.80 | Yes |
| 11.00090 | 0.000159536 | 250.049 | 0.20 | 0.80 | Yes |
| 10.00410 | 0.000176926 | 250.020 | 0.20 | 0.80 | Yes |
| 8.99881 | 0.000198925 | 250.046 | 0.20 | 0.80 | Yes |
| 8.00094 | 0.000226512 | 250.020 | 0.20 | 0.80 | Yes |
| 6.99772 | 0.000262783 | 250.048 | 0.20 | 0.80 | Yes |
| 6.01320 | 0.000310414 | 250.019 | 0.20 | 0.80 | Yes |
| 4.99748 | 0.000379943 | 250.044 | 0.20 | 0.80 | Yes |
| 4.03244 | 0.000478652 | 250.018 | 0.20 | 0.80 | Yes |
| 2.99627 | 0.000656238 | 250.044 | 0.20 | 0.80 | Yes |
| 1.97928 | 0.001012424 | 250.018 | 0.20 | 0.80 | Yes |
| 0.99791 | 0.002044948 | 250.046 | 0.20 | 0.80 | Yes |
| 0.99448 | 0.00205194 | 250.015 | 0.20 | 0.80 | Yes |
| 0.48824 | 0.004219278 | 250.046 | 0.20 | 0.80 | Yes |
| 19.42970 | 0.000107292 | 274.985 | 0.20 | 0.80 | Yes |
| 18.04310 | 0.000114724 | 274.986 | 0.20 | 0.80 | Yes |
| 16.00910 | 0.00012843 | 274.988 | 0.20 | 0.80 | Yes |
| 14.00570 | 0.000146519 | 274.989 | 0.20 | 0.80 | Yes |
| 12.00480 | 0.000171468 | 274.989 | 0.20 | 0.80 | Yes |
| 10.00030 | 0.000207508 | 274.991 | 0.20 | 0.80 | Yes |
| 7.99888 | 0.000262772 | 274.990 | 0.20 | 0.80 | Yes |
| 5.99721 | 0.000356429 | 274.991 | 0.20 | 0.80 | Yes |
| 3.99564 | 0.00054582 | 274.991 | 0.20 | 0.80 | Yes |
| 1.98781 | 0.0011225 | 274.989 | 0.20 | 0.80 | Yes |
| 0.99823 | 0.002261594 | 274.987 | 0.20 | 0.80 | Yes |
| 18.15090 | 0.000130668 | 299.954 | 0.20 | 0.80 | Yes |
| 17.07680 | 0.000138373 | 299.953 | 0.20 | 0.80 | Yes |
| 15.00170 | 0.000156717 | 299.951 | 0.20 | 0.80 | Yes |
| 13.03690 | 0.000180028 | 299.951 | 0.20 | 0.80 | Yes |
| 11.03220 | 0.000213038 | 299.950 | 0.20 | 0.80 | Yes |
| 8.99761 | 0.000262476 | 299.951 | 0.20 | 0.80 | Yes |
| 6.99712 | 0.000340141 | 299.951 | 0.20 | 0.80 | Yes |
| 4.99627 | 0.000481391 | 299.951 | 0.20 | 0.80 | Yes |
| 2.99620 | 0.000813057 | 299.953 | 0.20 | 0.80 | Yes |
| 0.98474 | 0.002512276 | 299.956 | 0.20 | 0.80 | Yes |
| 0.49288 | 0.005039561 | 299.957 | 0.20 | 0.80 | Yes |
| 19.96380 | 0.000134216 | 324.963 | 0.20 | 0.80 | Yes |
| 18.00200 | 0.000147592 | 324.962 | 0.20 | 0.80 | Yes |
| 16.00360 | 0.000164915 | 324.962 | 0.20 | 0.80 | Yes |
| 14.00150 | 0.000187624 | 324.961 | 0.20 | 0.80 | Yes |
| 12.00130 | 0.000218368 | 324.961 | 0.20 | 0.80 | Yes |
| 9.99931 | 0.000262035 | 324.960 | 0.20 | 0.80 | Yes |
| 7.99747 | 0.000328312 | 324.959 | 0.20 | 0.80 | Yes |
| 5.99710 | 0.000439664 | 324.960 | 0.20 | 0.80 | Yes |
| 3.97658 | 0.000667237 | 324.960 | 0.20 | 0.80 | Yes |
| 1.99409 | 0.0013415 | 324.960 | 0.20 | 0.80 | Yes |
| 1.99404 | 0.0013415 | 324.959 | 0.20 | 0.80 | Yes |
| 19.82050 | 0.000148952 | 349.948 | 0.20 | 0.80 | Yes |
| 17.99340 | 0.000162811 | 349.948 | 0.20 | 0.80 | Yes |
| 15.99920 | 0.000181802 | 349.948 | 0.20 | 0.80 | Yes |
| 13.99520 | 0.000206663 | 349.948 | 0.20 | 0.80 | Yes |
| 11.99640 | 0.000240121 | 349.948 | 0.20 | 0.80 | Yes |
| 9.97881 | 0.000287966 | 349.948 | 0.20 | 0.80 | Yes |
| 7.99624 | 0.000359107 | 349.949 | 0.20 | 0.80 | Yes |

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 5.99652 | 0.000479291 | 349.947 | 0.20 | 0.80 | Yes |
| 3.99594 | 0.000721068 | 349.948 | 0.20 | 0.80 | Yes |
| 1.99547 | 0.001450077 | 349.949 | 0.20 | 0.80 | Yes |
| 19.90270 | 0.000161719 | 374.942 | 0.20 | 0.80 | Yes |
| 17.84660 | 0.000178778 | 374.941 | 0.20 | 0.80 | Yes |
| 16.02340 | 0.000197761 | 374.942 | 0.20 | 0.80 | Yes |
| 13.98810 | 0.000225057 | 374.940 | 0.20 | 0.80 | Yes |
| 11.99000 | 0.000261196 | 374.941 | 0.20 | 0.80 | Yes |
| 9.99297 | 0.000312141 | 374.942 | 0.20 | 0.80 | Yes |
| 7.99534 | 0.00038907 | 374.941 | 0.20 | 0.80 | Yes |
| 5.99514 | 0.000518129 | 374.941 | 0.20 | 0.80 | Yes |
| 3.99570 | 0.000777238 | 374.940 | 0.20 | 0.80 | Yes |
| 1.99240 | 0.00156089 | 374.941 | 0.20 | 0.80 | Yes |
| 0.98192 | 0.003170137 | 374.940 | 0.20 | 0.80 | Yes |
| 19.97900 | 0.000174041 | 400.011 | 0.20 | 0.80 | Yes |
| 17.97910 | 0.000191741 | 400.012 | 0.20 | 0.80 | Yes |
| 15.98120 | 0.00021403 | 400.011 | 0.20 | 0.80 | Yes |
| 13.98660 | 0.000242857 | 400.012 | 0.20 | 0.80 | Yes |
| 11.98990 | 0.00028159 | 400.012 | 0.20 | 0.80 | Yes |
| 9.99056 | 0.00033622 | 400.012 | 0.20 | 0.80 | Yes |
| 7.99379 | 0.000418499 | 400.012 | 0.20 | 0.80 | Yes |
| 5.99466 | 0.000556358 | 400.012 | 0.20 | 0.80 | Yes |
| 3.99403 | 0.000833333 | 400.012 | 0.20 | 0.80 | Yes |
| 1.97816 | 0.001680668 | 400.010 | 0.20 | 0.80 | Yes |
| 0.99668 | 0.003335827 | 400.008 | 0.20 | 0.80 | Yes |
| 17.56300 | 8.44439E-05 | 275.039 | 0.50 | 0.50 | Yes |
| 17.02700 | 8.68477E-05 | 275.037 | 0.50 | 0.50 | Yes |
| 15.92570 | 9.26169E-05 | 275.029 | 0.50 | 0.50 | Yes |
| 15.03210 | 9.83165E-05 | 275.027 | 0.50 | 0.50 | Yes |
| 14.03160 | 0.000106097 | 275.027 | 0.50 | 0.50 | Yes |
| 13.02530 | 0.000115819 | 275.025 | 0.50 | 0.50 | Yes |
| 12.02510 | 0.000127903 | 275.025 | 0.50 | 0.50 | Yes |
| 11.01830 | 0.000143168 | 275.024 | 0.50 | 0.50 | Yes |
| 10.02880 | 0.000162084 | 275.023 | 0.50 | 0.50 | Yes |
| 9.12550 | 0.000183649 | 275.023 | 0.50 | 0.50 | Yes |
| 8.00600 | 0.000217945 | 275.023 | 0.50 | 0.50 | Yes |
| 7.00335 | 0.000258548 | 275.023 | 0.50 | 0.50 | Yes |
| 5.99952 | 0.000313185 | 275.023 | 0.50 | 0.50 | Yes |
| 4.99873 | 0.000389672 | 275.023 | 0.50 | 0.50 | Yes |
| 3.99739 | 0.000504525 | 275.024 | 0.50 | 0.50 | Yes |
| 2.99662 | 0.000695792 | 275.024 | 0.50 | 0.50 | Yes |
| 1.99331 | 0.001080635 | 275.023 | 0.50 | 0.50 | Yes |
| 0.99658 | 0.002228066 | 275.023 | 0.50 | 0.50 | Yes |
| 19.96960 | 9.34696E-05 | 299.971 | 0.50 | 0.50 | Yes |
| 19.02040 | 9.78291E-05 | 299.969 | 0.50 | 0.50 | Yes |
| 17.99720 | 0.000103247 | 299.969 | 0.50 | 0.50 | Yes |
| 16.99580 | 0.00010944 | 299.971 | 0.50 | 0.50 | Yes |
| 15.99850 | 0.000116666 | 299.965 | 0.50 | 0.50 | Yes |
| 14.99570 | 0.00012524 | 299.968 | 0.50 | 0.50 | Yes |
| 13.99620 | 0.000135376 | 299.968 | 0.50 | 0.50 | Yes |
| 12.99820 | 0.000147456 | 299.966 | 0.50 | 0.50 | Yes |
| 11.99480 | 0.00016205 | 299.968 | 0.50 | 0.50 | Yes |
| 10.99650 | 0.000179629 | 299.969 | 0.50 | 0.50 | Yes |
| 9.99650 | 0.000201219 | 299.973 | 0.50 | 0.50 | Yes |
| 9.99330 | 0.00020121 | 299.973 | 0.50 | 0.50 | Yes |
| 9.01433 | 0.000227481 | 299.970 | 0.50 | 0.50 | Yes |
| 8.00905 | 0.000261435 | 299.969 | 0.50 | 0.50 | Yes |
| 7.00490 | 0.000305428 | 299.969 | 0.50 | 0.50 | Yes |
| 6.02374 | 0.000362945 | 299.966 | 0.50 | 0.50 | Yes |
| 5.01581 | 0.000445751 | 299.967 | 0.50 | 0.50 | Yes |
| 4.00017 | 0.000571651 | 299.966 | 0.50 | 0.50 | Yes |
| 2.99882 | 0.000779522 | 299.966 | 0.50 | 0.50 | Yes |
| 1.99512 | 0.001197898 | 299.966 | 0.50 | 0.50 | Yes |
| 0.99587 | 0.002451995 | 299.964 | 0.50 | 0.50 | Yes |
| 19.43570 | 0.000114163 | 324.980 | 0.50 | 0.50 | Yes |
| 19.02310 | 0.000116608 | 324.980 | 0.50 | 0.50 | Yes |
| 18.01810 | 0.000123152 | 324.980 | 0.50 | 0.50 | Yes |
| 17.01240 | 0.000130659 | 324.980 | 0.50 | 0.50 | Yes |
| 16.01750 | 0.000139218 | 324.981 | 0.50 | 0.50 | Yes |
| 14.99080 | 0.000149467 | 324.981 | 0.50 | 0.50 | Yes |
| 14.01090 | 0.000160884 | 324.981 | 0.50 | 0.50 | Yes |
| 13.00840 | 0.000174594 | 324.982 | 0.50 | 0.50 | Yes |
| 12.00510 | 0.00019087 | 324.981 | 0.50 | 0.50 | Yes |
| 11.00120 | 0.000210385 | 324.980 | 0.50 | 0.50 | Yes |
| 10.00360 | 0.000233971 | 324.980 | 0.50 | 0.50 | Yes |
| 9.00191 | 0.000263181 | 324.981 | 0.50 | 0.50 | Yes |
| 7.99825 | 0.000300078 | 324.981 | 0.50 | 0.50 | Yes |
| 6.99807 | 0.000347644 | 324.981 | 0.50 | 0.50 | Yes |
| 5.99509 | 0.000411613 | 324.982 | 0.50 | 0.50 | Yes |
| 4.99725 | 0.00050103 | 324.982 | 0.50 | 0.50 | Yes |
| 3.99531 | 0.000636051 | 324.982 | 0.50 | 0.50 | Yes |
| 2.99643 | 0.000860865 | 324.983 | 0.50 | 0.50 | Yes |
| 1.99147 | 0.001315818 | 324.984 | 0.50 | 0.50 | Yes |
| 0.97407 | 0.002732999 | 324.983 | 0.50 | 0.50 | Yes |

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 19.97710 | 0.000127896 | 349.961 | 0.50 | 0.50 | Yes |
| 18.99730 | 0.000134393 | 349.962 | 0.50 | 0.50 | Yes |
| 17.99570 | 0.000141889 | 349.961 | 0.50 | 0.50 | Yes |
| 16.99630 | 0.000150384 | 349.961 | 0.50 | 0.50 | Yes |
| 15.99460 | 0.00016011 | 349.962 | 0.50 | 0.50 | Yes |
| 14.99750 | 0.00017124 | 349.962 | 0.50 | 0.50 | Yes |
| 14.00010 | 0.000184126 | 349.961 | 0.50 | 0.50 | Yes |
| 12.99820 | 0.000199235 | 349.961 | 0.50 | 0.50 | Yes |
| 11.99720 | 0.000217044 | 349.962 | 0.50 | 0.50 | Yes |
| 10.99770 | 0.000238232 | 349.961 | 0.50 | 0.50 | Yes |
| 9.99633 | 0.000263962 | 349.961 | 0.50 | 0.50 | Yes |
| 9.99633 | 0.000263962 | 349.961 | 0.50 | 0.50 | Yes |
| 8.99622 | 0.000295576 | 349.960 | 0.50 | 0.50 | Yes |
| 7.99547 | 0.000335354 | 349.960 | 0.50 | 0.50 | Yes |
| 6.99592 | 0.000386668 | 349.961 | 0.50 | 0.50 | Yes |
| 5.99622 | 0.000455396 | 349.961 | 0.50 | 0.50 | Yes |
| 4.99593 | 0.000551962 | 349.962 | 0.50 | 0.50 | Yes |
| 3.99702 | 0.000696963 | 349.962 | 0.50 | 0.50 | Yes |
| 2.99638 | 0.000939571 | 349.961 | 0.50 | 0.50 | Yes |
| 1.98830 | 0.001431695 | 349.962 | 0.50 | 0.50 | Yes |
| 0.98348 | 0.002926928 | 349.962 | 0.50 | 0.50 | Yes |
| 19.94080 | 0.000143787 | 374.953 | 0.50 | 0.50 | Yes |
| 19.11920 | 0.000149821 | 374.951 | 0.50 | 0.50 | Yes |
| 17.98780 | 0.000159158 | 374.953 | 0.50 | 0.50 | Yes |
| 16.99010 | 0.000168525 | 374.953 | 0.50 | 0.50 | Yes |
| 15.98960 | 0.000179206 | 374.953 | 0.50 | 0.50 | Yes |
| 14.99370 | 0.000191367 | 374.953 | 0.50 | 0.50 | Yes |
| 13.99470 | 0.000205437 | 374.954 | 0.50 | 0.50 | Yes |
| 12.99150 | 0.000221881 | 374.954 | 0.50 | 0.50 | Yes |
| 11.99250 | 0.000241136 | 374.953 | 0.50 | 0.50 | Yes |
| 10.99520 | 0.000263972 | 374.954 | 0.50 | 0.50 | Yes |
| 9.99586 | 0.000291647 | 374.953 | 0.50 | 0.50 | Yes |
| 9.99586 | 0.000291647 | 374.953 | 0.50 | 0.50 | Yes |
| 8.96527 | 0.000326811 | 374.953 | 0.50 | 0.50 | Yes |
| 8.05362 | 0.000365587 | 374.954 | 0.50 | 0.50 | Yes |
| 6.99503 | 0.000423493 | 374.952 | 0.50 | 0.50 | Yes |
| 5.99458 | 0.000497273 | 374.953 | 0.50 | 0.50 | Yes |
| 4.99326 | 0.000600988 | 374.952 | 0.50 | 0.50 | Yes |
| 3.99475 | 0.000756465 | 374.952 | 0.50 | 0.50 | Yes |
| 2.99568 | 0.001016112 | 374.953 | 0.50 | 0.50 | Yes |
| 1.98785 | 0.001543572 | 374.951 | 0.50 | 0.50 | Yes |
| 0.98706 | 0.003133484 | 374.954 | 0.50 | 0.50 | Yes |
| 19.96030 | 0.000158532 | 400.020 | 0.50 | 0.50 | Yes |
| 18.98310 | 0.000166446 | 400.018 | 0.50 | 0.50 | Yes |
| 17.96470 | 0.000175684 | 400.020 | 0.50 | 0.50 | Yes |
| 16.98380 | 0.00018572 | 400.018 | 0.50 | 0.50 | Yes |
| 15.98500 | 0.000197287 | 400.018 | 0.50 | 0.50 | Yes |
| 14.98390 | 0.000210523 | 400.019 | 0.50 | 0.50 | Yes |
| 13.98590 | 0.000225704 | 400.018 | 0.50 | 0.50 | Yes |
| 12.98370 | 0.000243403 | 400.019 | 0.50 | 0.50 | Yes |
| 11.98640 | 0.000264082 | 400.018 | 0.50 | 0.50 | Yes |
| 10.98740 | 0.000288655 | 400.019 | 0.50 | 0.50 | Yes |
| 9.97978 | 0.000318622 | 400.019 | 0.50 | 0.50 | Yes |
| 9.97978 | 0.000318622 | 400.019 | 0.50 | 0.50 | Yes |
| 8.99459 | 0.00035453 | 400.017 | 0.50 | 0.50 | Yes |
| 7.99241 | 0.000400307 | 400.018 | 0.50 | 0.50 | Yes |
| 6.99141 | 0.000459282 | 400.019 | 0.50 | 0.50 | Yes |
| 5.99420 | 0.000537864 | 400.020 | 0.50 | 0.50 | Yes |
| 4.99316 | 0.000648513 | 400.020 | 0.50 | 0.50 | Yes |
| 3.98088 | 0.000817332 | 400.019 | 0.50 | 0.50 | Yes |
| 2.99564 | 0.001091477 | 400.018 | 0.50 | 0.50 | Yes |
| 1.98761 | 0.001654339 | 400.019 | 0.50 | 0.50 | Yes |
| 0.97589 | 0.003388858 | 400.018 | 0.50 | 0.50 | Yes |

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{N_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 19.94 | 0.00028586 | 673.15 | 0.9 | 0.1 | Yes |
| 29.94 | 0.00019486 | 673.15 | 0.9 | 0.1 | Yes |
| 39.94 | 0.00015053 | 673.15 | 0.9 | 0.1 | Yes |
| 79.93 | 0.00008816 | 673.15 | 0.9 | 0.1 | Yes |
| 19.94 | 0.00028796 | 673.15 | 0.8 | 0.2 | Yes |
| 29.94 | 0.00019706 | 673.15 | 0.8 | 0.2 | Yes |
| 39.94 | 0.00015290 | 673.15 | 0.8 | 0.2 | Yes |
| 59.93 | 0.00010985 | 673.15 | 0.8 | 0.2 | Yes |
| 79.93 | 0.00008948 | 673.15 | 0.8 | 0.2 | Yes |
| 99.93 | 0.00007760 | 673.15 | 0.8 | 0.2 | Yes |
| 19.94 | 0.00029161 | 673.15 | 0.7 | 0.3 | Yes |
| 29.94 | 0.00019967 | 673.15 | 0.7 | 0.3 | Yes |
| 39.94 | 0.00015471 | 673.15 | 0.7 | 0.3 | Yes |
| 59.93 | 0.00011156 | 673.15 | 0.7 | 0.3 | Yes |
| 79.93 | 0.00009073 | 673.15 | 0.7 | 0.3 | Yes |
| 99.93 | 0.00007862 | 673.15 | 0.7 | 0.3 | Yes |
| 19.94 | 0.00029426 | 673.15 | 0.6 | 0.4 | Yes |
| 29.94 | 0.00020190 | 673.15 | 0.6 | 0.4 | Yes |
| 39.94 | 0.00015677 | 673.15 | 0.6 | 0.4 | Yes |
| 59.93 | 0.00011306 | 673.15 | 0.6 | 0.4 | Yes |
| 79.93 | 0.00009197 | 673.15 | 0.6 | 0.4 | Yes |
| 99.93 | 0.00007953 | 673.15 | 0.6 | 0.4 | Yes |
| 19.94 | 0.00029657 | 673.15 | 0.5 | 0.5 | Yes |
| 29.94 | 0.00020376 | 673.15 | 0.5 | 0.5 | Yes |
| 39.94 | 0.00015852 | 673.15 | 0.5 | 0.5 | Yes |
| 59.93 | 0.00011451 | 673.15 | 0.5 | 0.5 | Yes |
| 79.93 | 0.00009310 | 673.15 | 0.5 | 0.5 | Yes |
| 99.93 | 0.00008047 | 673.15 | 0.5 | 0.5 | Yes |
| 19.94 | 0.00029940 | 673.15 | 0.4 | 0.6 | Yes |
| 29.94 | 0.00020592 | 673.15 | 0.4 | 0.6 | Yes |
| 39.94 | 0.00016034 | 673.15 | 0.4 | 0.6 | Yes |
| 59.93 | 0.00011598 | 673.15 | 0.4 | 0.6 | Yes |
| 79.93 | 0.00009416 | 673.15 | 0.4 | 0.6 | Yes |
| 99.93 | 0.00008130 | 673.15 | 0.4 | 0.6 | Yes |
| 19.94 | 0.00030134 | 673.15 | 0.3 | 0.7 | Yes |
| 29.94 | 0.00020768 | 673.15 | 0.3 | 0.7 | Yes |
| 39.94 | 0.00016214 | 673.15 | 0.3 | 0.7 | Yes |
| 59.93 | 0.00011724 | 673.15 | 0.3 | 0.7 | Yes |
| 79.93 | 0.00009520 | 673.15 | 0.3 | 0.7 | Yes |
| 99.93 | 0.00008204 | 673.15 | 0.3 | 0.7 | Yes |
| 19.94 | 0.00030325 | 673.15 | 0.2 | 0.8 | Yes |
| 29.94 | 0.00020911 | 673.15 | 0.2 | 0.8 | Yes |
| 39.94 | 0.00016343 | 673.15 | 0.2 | 0.8 | Yes |
| 59.93 | 0.00011837 | 673.15 | 0.2 | 0.8 | Yes |
| 79.93 | 0.00009609 | 673.15 | 0.2 | 0.8 | Yes |
| 99.93 | 0.00008274 | 673.15 | 0.2 | 0.8 | Yes |
| 19.94 | 0.00030523 | 673.15 | 0.1 | 0.9 | Yes |
| 29.94 | 0.00021085 | 673.15 | 0.1 | 0.9 | Yes |
| 59.93 | 0.00011940 | 673.15 | 0.1 | 0.9 | Yes |
| 79.93 | 0.00009701 | 673.15 | 0.1 | 0.9 | Yes |
| 99.93 | 0.00008333 | 673.15 | 0.1 | 0.9 | Yes |

Data summarised from TABLE 3 of Seitz96 [81]

7.1.3 Carbon Dioxide–Hydrogen VLE Data

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | y_{CO_2} | y_{H_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 4.805 | 7.29286E-05 | — | 278.15 | 0.9912 | 0.0088 | 0.8861 | 0.1139 | Vol. Est. |
| 5.864 | 7.06064E-05 | — | 278.15 | 0.9798 | 0.0202 | 0.8158 | 0.1842 | Vol. Est. |
| 6.933 | 7.16311E-05 | — | 278.15 | 0.9751 | 0.0249 | 0.7467 | 0.2533 | Vol. Est. |
| 7.722 | 8.58936E-05 | — | 278.15 | 0.971 | 0.029 | 0.7211 | 0.2789 | Vol. Est. |
| 8.671 | 8.08698E-05 | — | 278.15 | 0.9555 | 0.0445 | 0.6963 | 0.3037 | Vol. Est. |
| 9.961 | 7.8573E-05 | — | 278.15 | 0.9386 | 0.0614 | 0.6589 | 0.3411 | Vol. Est. |
| 10.86 | 7.56868E-05 | — | 278.15 | 0.9339 | 0.0661 | 0.6419 | 0.3581 | Vol. Est. |
| 11.4 | 7.74803E-05 | — | 278.15 | 0.9282 | 0.0718 | 0.6238 | 0.3762 | Vol. Est. |
| 11.77 | 7.48026E-05 | — | 278.15 | 0.9251 | 0.0749 | 0.6182 | 0.3818 | Vol. Est. |
| 12.6 | 7.73807E-05 | — | 278.15 | 0.9181 | 0.0819 | 0.5898 | 0.4102 | Vol. Est. |
| 13.688 | 7.74632E-05 | — | 278.15 | 0.9088 | 0.0912 | 0.5669 | 0.4331 | Vol. Est. |
| 14.487 | 7.5925E-05 | — | 278.15 | 0.903 | 0.097 | 0.5493 | 0.4507 | Vol. Est. |
| 15.367 | 7.51067E-05 | — | 278.15 | 0.8974 | 0.1026 | 0.5204 | 0.4796 | Vol. Est. |
| 16.985 | 7.37238E-05 | — | 278.15 | 0.8821 | 0.1179 | 0.4962 | 0.5038 | Vol. Est. |
| 18.68 | 7.21551E-05 | — | 278.15 | 0.8709 | 0.1291 | 0.4958 | 0.5042 | Vol. Est. |
| 19.253 | 7.22321E-05 | — | 278.15 | 0.8693 | 0.1307 | 0.4945 | 0.5055 | Vol. Est. |
| 6.174 | 7.68363E-05 | — | 290.15 | 0.9887 | 0.0113 | 0.9505 | 0.0495 | Vol. Est. |
| 7.1 | 7.5917E-05 | — | 290.15 | 0.9772 | 0.0228 | 0.9021 | 0.0979 | Vol. Est. |
| 8.392 | 8.51229E-05 | — | 290.15 | 0.9651 | 0.0349 | 0.8444 | 0.1556 | Vol. Est. |
| 9.23 | 8.3795E-05 | — | 290.15 | 0.9477 | 0.0523 | 0.7944 | 0.2056 | Vol. Est. |
| 9.31 | 8.02502E-05 | — | 290.15 | 0.9459 | 0.0541 | 0.7811 | 0.2189 | Vol. Est. |
| 9.79 | 8.01922E-05 | — | 290.15 | 0.9427 | 0.0573 | 0.7611 | 0.2389 | Vol. Est. |
| 9.93 | 7.34361E-05 | — | 290.15 | 0.9395 | 0.0605 | — | — | No |
| 10.37 | 7.35931E-05 | — | 290.15 | 0.9339 | 0.0661 | — | — | No |
| 10.93 | 7.78437E-05 | — | 290.15 | 0.9287 | 0.0713 | — | — | No |
| 11.62 | 7.78023E-05 | — | 290.15 | 0.9204 | 0.0796 | 0.7265 | 0.2735 | Vol. Est. |
| 12.38 | 7.85079E-05 | — | 290.15 | 0.9103 | 0.0897 | 0.718 | 0.282 | Vol. Est. |
| 13.29 | 7.69746E-05 | — | 290.15 | 0.8969 | 0.1031 | 0.7082 | 0.2918 | Vol. Est. |
| 13.558 | 7.51758E-05 | — | 290.15 | 0.8963 | 0.1037 | — | — | No |
| 14.547 | 7.46894E-05 | — | 290.15 | 0.8861 | 0.1139 | — | — | No |
| 14.997 | 7.58879E-05 | — | 290.15 | 0.8785 | 0.1215 | — | — | No |
| 16.026 | 7.61376E-05 | — | 290.15 | 0.8636 | 0.1364 | 0.6799 | 0.3201 | Vol. Est. |
| 17.565 | 7.49539E-05 | — | 290.15 | 0.8455 | 0.1545 | 0.6638 | 0.3362 | Vol. Est. |
| 18.394 | 7.38506E-05 | — | 290.15 | 0.8429 | 0.1571 | 0.6771 | 0.3229 | Vol. Est. |
| 7.193 | 7.84861E-05 | — | 298.15 | 0.9904 | 0.0096 | 0.9575 | 0.0425 | Vol. Est. |
| 8.02 | 7.66238E-05 | — | 298.15 | 0.9716 | 0.0284 | 0.9257 | 0.0743 | Vol. Est. |
| 8.592 | 7.97702E-05 | — | 298.15 | 0.9618 | 0.0382 | 0.8994 | 0.1006 | Vol. Est. |
| 9.061 | 7.79605E-05 | — | 298.15 | 0.9556 | 0.0444 | 0.8667 | 0.1333 | Vol. Est. |
| 9.57 | 7.86966E-05 | — | 298.15 | 0.9439 | 0.0561 | 0.8391 | 0.1609 | Vol. Est. |
| 11.09 | 7.94229E-05 | — | 298.15 | 0.9192 | 0.0808 | 0.8062 | 0.1938 | Vol. Est. |
| 11.39 | 8.0662E-05 | — | 298.15 | 0.9122 | 0.0878 | — | — | No |
| 11.59 | 7.92922E-05 | — | 298.15 | 0.911 | 0.089 | — | — | No |

Data summarised from Table 4 of Bezanehtak02 [90]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | y_{CO_2} | y_{H_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 6.909 | — | 0.000278 | 258.15 | — | — | 0.448 | 0.552 | No |
| 6.915 | 0.0000439 | 0.000286 | 258.15 | 0.976 | 0.024 | 0.449 | 0.551 | Vol. Est. |
| 13.789 | 0.0000432 | 0.000154 | 258.15 | 0.9405 | 0.0595 | 0.299 | 0.701 | Vol. Est. |
| 27.558 | 0.000042 | 0.0000847 | 258.15 | 0.868 | 0.132 | 0.242 | 0.758 | Vol. Est. |
| 6.895 | 0.0000474 | 0.000258 | 273.15 | 0.9734 | 0.0266 | 0.6385 | 0.3615 | Vol. Est. |
| 13.796 | 0.0000467 | 0.000145 | 273.15 | 0.9201 | 0.0799 | 0.45 | 0.55 | Vol. Est. |
| 27.607 | 0.0000457 | 0.0000806 | 273.15 | 0.807 | 0.193 | 0.39 | 0.61 | Vol. Est. |

Data summarised from TABLE 1 and 2 of Freitag86 [92]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{H_2} | y_{CO_2} | y_{H_2} | Usable Data Point? |
|-----------|---|---|---------------|-------------------|------------------|-------------------|------------------|--------------------|
| 2.04 | — | — | 252.80 | — | — | 0.9699 | 0.0301 | No |
| 8 | — | — | 252.80 | 0.9699 | 0.0301 | — | — | No |
| 7.96 | — | — | 257.82 | 0.9699 | 0.0301 | — | — | No |
| 2.38 | — | — | 257.83 | — | — | 0.9699 | 0.0301 | No |
| 2.76 | — | — | 262.79 | — | — | 0.9699 | 0.0301 | No |
| 7.76 | — | — | 262.81 | 0.9699 | 0.0301 | — | — | No |
| 3.17 | — | — | 267.76 | — | — | 0.9699 | 0.0301 | No |
| 7.75 | — | — | 267.78 | 0.9699 | 0.0301 | — | — | No |
| 3.63 | — | — | 272.74 | — | — | 0.9699 | 0.0301 | No |
| 7.76 | — | — | 272.74 | 0.9699 | 0.0301 | — | — | No |
| 10.56 | — | — | 272.97 | 0.9501 | 0.0499 | — | — | No |
| 3.76 | — | — | 273.00 | — | — | 0.9501 | 0.0499 | No |
| 10.48 | — | — | 274.00 | 0.9501 | 0.0499 | — | — | No |
| 10.34 | — | — | 275.89 | 0.9501 | 0.0499 | — | — | No |
| 4.19 | — | — | 276.98 | — | — | 0.9501 | 0.0499 | No |
| 7.78 | — | — | 277.79 | 0.9699 | 0.0301 | — | — | No |
| 4.16 | — | — | 277.81 | — | — | 0.9699 | 0.0301 | No |
| 10.35 | — | — | 277.95 | 0.9501 | 0.0499 | — | — | No |
| 10.25 | — | — | 280.95 | 0.9501 | 0.0499 | — | — | No |
| 4.66 | — | — | 280.98 | — | — | 0.9501 | 0.0499 | No |
| 7.98 | — | — | 282.78 | 0.9699 | 0.0301 | — | — | No |
| 4.75 | — | — | 282.86 | — | — | 0.9699 | 0.0301 | No |
| 10.26 | — | — | 282.95 | 0.9501 | 0.0499 | — | — | No |
| 5.18 | — | — | 284.97 | — | — | 0.9501 | 0.0499 | No |
| 10.21 | — | — | 284.97 | 0.9501 | 0.0499 | — | — | No |
| 7.98 | — | — | 285.32 | 0.9699 | 0.0301 | — | — | No |
| 5.32 | — | — | 285.98 | — | — | 0.9501 | 0.0499 | No |
| 8.18 | — | — | 287.82 | 0.9699 | 0.0301 | — | — | No |
| 5.38 | — | — | 287.83 | — | — | 0.9699 | 0.0301 | No |
| 10.18 | — | — | 287.96 | 0.9501 | 0.0499 | — | — | No |
| 5.75 | — | — | 288.97 | — | — | 0.9501 | 0.0499 | No |
| 10.06 | — | — | 289.94 | 0.9501 | 0.0499 | — | — | No |
| 5.73 | — | — | 290.30 | — | — | 0.9699 | 0.0301 | No |
| 8.26 | — | — | 290.35 | 0.9699 | 0.0301 | — | — | No |
| 8.36 | — | — | 292.80 | 0.9699 | 0.0301 | — | — | No |
| 6.08 | — | — | 292.81 | — | — | 0.9699 | 0.0301 | No |
| 10.1 | — | — | 292.97 | 0.9501 | 0.0499 | — | — | No |
| 6.39 | — | — | 292.98 | — | — | 0.9501 | 0.0499 | No |
| 10.03 | — | — | 294.96 | 0.9501 | 0.0499 | — | — | No |
| 6.47 | — | — | 295.34 | — | — | 0.9699 | 0.0301 | No |
| 8.47 | — | — | 295.34 | 0.9699 | 0.0301 | — | — | No |
| 6.84 | — | — | 295.49 | — | — | 0.9501 | 0.0499 | No |
| 8.57 | — | — | 296.36 | 0.9699 | 0.0301 | — | — | No |
| 9.99 | — | — | 296.42 | 0.9501 | 0.0499 | — | — | No |
| 8.6 | — | — | 297.83 | 0.9699 | 0.0301 | — | — | No |
| 6.91 | — | — | 297.84 | — | — | 0.9699 | 0.0301 | No |
| 7.35 | — | — | 297.99 | — | — | 0.9501 | 0.0499 | No |
| 9.92 | — | — | 297.99 | 0.9501 | 0.0499 | — | — | No |
| 7.08 | — | — | 298.83 | — | — | 0.9699 | 0.0301 | No |
| 8.72 | — | — | 298.83 | 0.9699 | 0.0301 | — | — | No |
| 9.88 | — | — | 299.00 | 0.9501 | 0.0499 | — | — | No |
| 7.7 | — | — | 299.49 | — | — | 0.9501 | 0.0499 | No |
| 7.29 | — | — | 299.86 | — | — | 0.9699 | 0.0301 | No |
| 9.73 | — | — | 299.98 | 0.9501 | 0.0499 | — | — | No |
| 8.68 | — | — | 300.34 | 0.9699 | 0.0301 | — | — | No |
| 7.43 | — | — | 300.40 | — | — | 0.9699 | 0.0301 | No |
| 7.99 | — | — | 300.48 | — | — | 0.9501 | 0.0499 | No |
| 7.53 | — | — | 300.86 | — | — | 0.9699 | 0.0301 | No |
| 8.12 | — | — | 300.98 | — | — | 0.9501 | 0.0499 | No |
| 9.59 | — | — | 300.98 | 0.9501 | 0.0499 | — | — | No |
| 7.63 | — | — | 301.38 | — | — | 0.9699 | 0.0301 | No |
| 8.21 | — | — | 301.48 | — | — | 0.9501 | 0.0499 | No |
| 9.39 | — | — | 301.48 | 0.9501 | 0.0499 | — | — | No |
| 8.62 | — | — | 301.86 | 0.9699 | 0.0301 | — | — | No |
| 7.76 | — | — | 301.88 | — | — | 0.9699 | 0.0301 | No |
| 8.36 | — | — | 301.96 | — | — | 0.9501 | 0.0499 | No |
| 9.19 | — | — | 301.99 | 0.9501 | 0.0499 | — | — | No |
| 8.59 | — | — | 302.11 | 0.9699 | 0.0301 | — | — | No |
| 8.54 | — | — | 302.22 | — | — | 0.9501 | 0.0499 | No |
| 8.96 | — | — | 302.23 | 0.9501 | 0.0499 | — | — | No |
| 8.81 | — | — | 302.41 | — | — | 0.9501 | 0.0499 | No |
| 7.88 | — | — | 302.42 | — | — | 0.9699 | 0.0301 | No |
| 8.32 | — | — | 302.87 | — | — | — | — | No |

Data summarised from Table 1 and 2 of Parrott13 [121]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | y_{CO_2} | y_{H_2} | Usable Data Point? |
|-----------|---|---|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 0.93 | — | — | 220 | 0.9985 | 0.0015 | 0.7102 | 0.2898 | Vol. Est. |
| 1.00 | — | — | 220 | — | — | 0.6555 | 0.3445 | No |
| 1.07 | — | — | 220 | 0.9972 | 0.0028 | 0.6129 | 0.3871 | Vol. Est. |
| 1.18 | — | — | 220 | — | — | 0.5691 | 0.4309 | No |
| 1.27 | — | — | 220 | 0.9968 | 0.0032 | 0.5358 | 0.4642 | Vol. Est. |
| 1.35 | — | — | 220 | 0.9965 | 0.0035 | 0.4975 | 0.5025 | Vol. Est. |
| 2.23 | — | — | 220 | 0.9933 | 0.0067 | 0.3245 | 0.6755 | Vol. Est. |
| 3.51 | — | — | 220 | 0.9888 | 0.0112 | 0.2190 | 0.7810 | Vol. Est. |
| 5.13 | — | — | 220 | 0.9841 | 0.0159 | 0.1631 | 0.8369 | Vol. Est. |
| 7.13 | — | — | 220 | 0.9782 | 0.0218 | 0.1263 | 0.8737 | Vol. Est. |
| 11.01 | — | — | 220 | 0.9703 | 0.0297 | 0.0945 | 0.9055 | Vol. Est. |
| 14.00 | — | — | 220 | 0.9639 | 0.0361 | 0.0838 | 0.9162 | Vol. Est. |
| 15.46 | — | — | 220 | 0.9606 | 0.0394 | 0.0811 | 0.9189 | Vol. Est. |
| 16.93 | — | — | 220 | 0.9573 | 0.0427 | 0.0787 | 0.9213 | Vol. Est. |
| 18.79 | — | — | 220 | 0.9537 | 0.0463 | 0.0791 | 0.9209 | Vol. Est. |
| 20.99 | — | — | 220 | 0.9486 | 0.0514 | 0.0740 | 0.9260 | Vol. Est. |
| 24.34 | — | — | 220 | 0.9407 | 0.0593 | 0.0701 | 0.9299 | Vol. Est. |
| 26.44 | — | — | 220 | 0.9353 | 0.0647 | 0.0693 | 0.9307 | Vol. Est. |
| 27.59 | — | — | 220 | 0.9337 | 0.0663 | 0.0697 | 0.9303 | Vol. Est. |
| 31.50 | — | — | 220 | 0.9279 | 0.0721 | 0.0693 | 0.9307 | Vol. Est. |
| 35.40 | — | — | 220 | 0.9162 | 0.0838 | 0.0685 | 0.9315 | Vol. Est. |
| 1.18 | — | — | 225 | 0.9977 | 0.0023 | 0.6898 | 0.3102 | Vol. Est. |
| 1.47 | — | — | 225 | 0.9961 | 0.0039 | 0.5628 | 0.4372 | Vol. Est. |
| 1.49 | — | — | 225 | 0.9961 | 0.0039 | 0.7873 | 0.2127 | Vol. Est. |
| 2.14 | — | — | 225 | 0.9931 | 0.0069 | 0.5772 | 0.4228 | Vol. Est. |
| 2.16 | — | — | 225 | 0.9932 | 0.0068 | 0.4003 | 0.5997 | Vol. Est. |
| 2.78 | — | — | 225 | 0.9911 | 0.0089 | 0.3243 | 0.6757 | Vol. Est. |
| 3.38 | — | — | 225 | 0.9879 | 0.0121 | 0.3912 | 0.6088 | Vol. Est. |
| 3.56 | — | — | 225 | 0.9883 | 0.0117 | 0.2591 | 0.7409 | Vol. Est. |
| 4.85 | — | — | 225 | 0.9841 | 0.0159 | 0.2035 | 0.7965 | Vol. Est. |
| 5.22 | — | — | 225 | 0.9815 | 0.0185 | 0.2714 | 0.7286 | Vol. Est. |
| 7.00 | — | — | 225 | 0.9782 | 0.0218 | 0.1493 | 0.8507 | Vol. Est. |
| 7.06 | — | — | 225 | 0.9757 | 0.0243 | 0.2194 | 0.7806 | Vol. Est. |
| 10.46 | — | — | 225 | 0.9658 | 0.0342 | 0.1678 | 0.8322 | Vol. Est. |
| 10.65 | — | — | 225 | 0.9688 | 0.0312 | 0.1110 | 0.8890 | Vol. Est. |
| 14.03 | — | — | 225 | 0.9550 | 0.0450 | 0.1438 | 0.8562 | Vol. Est. |
| 14.22 | — | — | 225 | 0.9607 | 0.0393 | 0.0964 | 0.9036 | Vol. Est. |
| 20.73 | — | — | 225 | 0.9341 | 0.0659 | 0.1245 | 0.8755 | Vol. Est. |
| 21.15 | — | — | 225 | 0.9433 | 0.0567 | 0.0822 | 0.9178 | Vol. Est. |
| 27.71 | — | — | 225 | 0.9119 | 0.0881 | 0.3172 | 0.6828 | Vol. Est. |
| 27.88 | — | — | 225 | 0.9260 | 0.0740 | 0.0775 | 0.9225 | Vol. Est. |
| 34.69 | — | — | 225 | 0.9086 | 0.0914 | 0.0768 | 0.9232 | Vol. Est. |
| 35.22 | — | — | 225 | 0.8877 | 0.1123 | 0.1132 | 0.8868 | Vol. Est. |
| 41.38 | — | — | 225 | 0.8693 | 0.1307 | 0.1136 | 0.8864 | Vol. Est. |
| 41.44 | — | — | 225 | 0.8927 | 0.1073 | 0.0760 | 0.9240 | Vol. Est. |
| 48.37 | — | — | 225 | 0.8765 | 0.1235 | 0.0772 | 0.9228 | Vol. Est. |
| 55.17 | — | — | 225 | 0.8293 | 0.1707 | 0.1187 | 0.8813 | Vol. Est. |
| 55.35 | — | — | 225 | 0.8610 | 0.1390 | 0.0791 | 0.9209 | Vol. Est. |
| 69.99 | — | — | 225 | 0.8310 | 0.1690 | 0.0869 | 0.9131 | Vol. Est. |
| 73.10 | — | — | 225 | 0.7816 | 0.2184 | 0.1296 | 0.8704 | Vol. Est. |
| 79.48 | — | — | 225 | 0.8123 | 0.1877 | 0.0930 | 0.9070 | Vol. Est. |
| 91.26 | — | — | 225 | 0.7888 | 0.2112 | 0.0964 | 0.9036 | Vol. Est. |
| 93.03 | — | — | 225 | 0.7272 | 0.2728 | 0.1438 | 0.8562 | Vol. Est. |
| 117.61 | — | — | 225 | 0.6629 | 0.3371 | 0.1657 | 0.8343 | Vol. Est. |
| 137.35 | — | — | 225 | 0.6072 | 0.3928 | 0.1898 | 0.8102 | Vol. Est. |
| 152.00 | — | — | 225 | 0.5635 | 0.4365 | 0.2123 | 0.7877 | Vol. Est. |
| 165.58 | — | — | 225 | 0.5116 | 0.4884 | 0.2444 | 0.7556 | Vol. Est. |
| 168.96 | — | — | 225 | 0.4938 | 0.5062 | 0.2545 | 0.7455 | Vol. Est. |
| 171.79 | — | — | 225 | 0.4736 | 0.5264 | 0.2672 | 0.7328 | Vol. Est. |
| 132.08 | — | — | 237 | 0.5933 | 0.4067 | 0.2051 | 0.7949 | Vol. Est. |
| 138.00 | — | — | 237 | 0.5719 | 0.4281 | 0.2163 | 0.7837 | Vol. Est. |
| 144.90 | — | — | 237 | 0.5470 | 0.4530 | 0.2302 | 0.7698 | Vol. Est. |
| 148.35 | — | — | 237 | 0.5269 | 0.4731 | 0.2476 | 0.7524 | Vol. Est. |
| 150.28 | — | — | 237 | 0.5211 | 0.4789 | 0.2514 | 0.7486 | Vol. Est. |
| 152.07 | — | — | 237 | 0.5092 | 0.4908 | 0.2610 | 0.7390 | Vol. Est. |
| 154.90 | — | — | 237 | 0.4951 | 0.5049 | 0.2700 | 0.7300 | Vol. Est. |
| 156.97 | — | — | 237 | 0.4762 | 0.5238 | 0.2810 | 0.7190 | Vol. Est. |
| 158.83 | — | — | 237 | 0.4599 | 0.5401 | 0.2954 | 0.7046 | Vol. Est. |
| 160.41 | — | — | 237 | 0.4434 | 0.5566 | 0.3079 | 0.6921 | Vol. Est. |
| 83.68 | — | — | 245 | 0.6749 | 0.3251 | 0.2082 | 0.7918 | Vol. Est. |
| 89.58 | — | — | 245 | 0.6479 | 0.3521 | 0.2224 | 0.7776 | Vol. Est. |
| 96.65 | — | — | 245 | 0.6118 | 0.3882 | 0.2400 | 0.7600 | Vol. Est. |
| 101.54 | — | — | 245 | 0.5845 | 0.4155 | 0.2559 | 0.7441 | Vol. Est. |
| 105.06 | — | — | 245 | 0.5621 | 0.4379 | 0.2697 | 0.7303 | Vol. Est. |
| 108.51 | — | — | 245 | 0.5343 | 0.4657 | 0.2906 | 0.7094 | Vol. Est. |
| 111.83 | — | — | 245 | 0.4990 | 0.5010 | 0.3211 | 0.6789 | Vol. Est. |
| 113.23 | — | — | 245 | 0.4738 | 0.5262 | 0.3397 | 0.6603 | Vol. Est. |

Data summarised from Table 1 of Tsang81 [110]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | y_{CO_2} | y_{H_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 2.31 | — | — | 250 | 0.9956 | 0.0044 | 0.8411 | 0.1589 | Vol. Est. |
| 3.04 | — | — | 250 | 0.9914 | 0.0086 | 0.6804 | 0.3196 | Vol. Est. |
| 3.63 | — | — | 250 | 0.9876 | 0.0124 | 0.5910 | 0.4090 | Vol. Est. |
| 5.20 | — | — | 250 | 0.9814 | 0.0186 | 0.4499 | 0.5501 | Vol. Est. |
| 6.90 | — | — | 250 | 0.9738 | 0.0262 | 0.3629 | 0.6371 | Vol. Est. |
| 10.29 | — | — | 250 | 0.9604 | 0.0396 | 0.2821 | 0.7179 | Vol. Est. |
| 13.85 | — | — | 250 | 0.9455 | 0.0545 | 0.2415 | 0.7585 | Vol. Est. |
| 17.28 | — | — | 250 | 0.9305 | 0.0695 | 0.2178 | 0.7822 | Vol. Est. |
| 25.44 | — | — | 250 | 0.8942 | 0.1058 | 0.1956 | 0.8044 | Vol. Est. |
| 31.54 | — | — | 250 | 0.8668 | 0.1332 | 0.1895 | 0.8105 | Vol. Est. |
| 35.34 | — | — | 250 | 0.8512 | 0.1488 | 0.1884 | 0.8116 | Vol. Est. |
| 49.66 | — | — | 250 | 0.7879 | 0.2121 | 0.1940 | 0.8060 | Vol. Est. |
| 62.81 | — | — | 250 | 0.7276 | 0.2724 | 0.2166 | 0.7834 | Vol. Est. |
| 75.88 | — | — | 250 | 0.6588 | 0.3412 | 0.2459 | 0.7541 | Vol. Est. |
| 83.22 | — | — | 250 | 0.6113 | 0.3887 | 0.2700 | 0.7300 | Vol. Est. |
| 86.54 | — | — | 250 | 0.5853 | 0.4147 | 0.2874 | 0.7126 | Vol. Est. |
| 88.39 | — | — | 250 | 0.5683 | 0.4317 | 0.2970 | 0.7030 | Vol. Est. |
| 91.61 | — | — | 250 | 0.5320 | 0.4680 | — | — | No |
| 3.37 | — | — | 260 | 0.9919 | 0.0081 | 0.7917 | 0.2083 | Vol. Est. |
| 4.38 | — | — | 260 | 0.9882 | 0.0118 | 0.8232 | 0.1768 | Vol. Est. |
| 5.31 | — | — | 260 | 0.9809 | 0.0191 | 0.7251 | 0.2749 | Vol. Est. |
| 5.58 | — | — | 260 | 0.9792 | 0.0208 | 0.5489 | 0.4511 | Vol. Est. |
| 7.08 | — | — | 260 | 0.9699 | 0.0301 | 0.6029 | 0.3971 | Vol. Est. |
| 7.23 | — | — | 260 | 0.9716 | 0.0284 | 0.4618 | 0.5382 | Vol. Est. |
| 10.53 | — | — | 260 | 0.9550 | 0.0450 | 0.3652 | 0.6348 | Vol. Est. |
| 10.62 | — | — | 260 | 0.9436 | 0.0564 | 0.4718 | 0.5282 | Vol. Est. |
| 13.49 | — | — | 260 | 0.9404 | 0.0596 | 0.3213 | 0.6787 | Vol. Est. |
| 13.86 | — | — | 260 | 0.9183 | 0.0817 | 0.4148 | 0.5852 | Vol. Est. |
| 17.44 | — | — | 260 | 0.8905 | 0.1095 | 0.3799 | 0.6201 | Vol. Est. |
| 21.62 | — | — | 260 | 0.8956 | 0.1044 | 0.2658 | 0.7342 | Vol. Est. |
| 21.93 | — | — | 260 | 0.8612 | 0.1388 | 0.3560 | 0.6440 | Vol. Est. |
| 25.26 | — | — | 260 | 0.8294 | 0.1706 | 0.3504 | 0.6496 | Vol. Est. |
| 27.97 | — | — | 260 | 0.8044 | 0.1956 | 0.3525 | 0.6475 | Vol. Est. |
| 28.15 | — | — | 260 | 0.8586 | 0.1414 | 0.2517 | 0.7483 | Vol. Est. |
| 34.70 | — | — | 260 | 0.8223 | 0.1777 | 0.2517 | 0.7483 | Vol. Est. |
| 34.76 | — | — | 260 | 0.7543 | 0.2457 | 0.3601 | 0.6399 | Vol. Est. |
| 39.99 | — | — | 260 | 0.7050 | 0.2950 | 0.3843 | 0.6157 | Vol. Est. |
| 41.71 | — | — | 260 | 0.7803 | 0.2197 | 0.2630 | 0.7370 | Vol. Est. |
| 44.14 | — | — | 260 | 0.6440 | 0.3560 | 0.4249 | 0.5751 | Vol. Est. |
| 45.69 | — | — | 260 | 0.6033 | 0.3967 | 0.4668 | 0.5332 | Vol. Est. |
| 48.44 | — | — | 260 | 0.7360 | 0.2640 | 0.2783 | 0.7217 | Vol. Est. |
| 55.59 | — | — | 260 | 0.6801 | 0.3199 | 0.3035 | 0.6965 | Vol. Est. |
| 62.04 | — | — | 260 | 0.6092 | 0.3908 | 0.3529 | 0.6471 | Vol. Est. |
| 65.64 | — | — | 260 | 0.5232 | 0.4768 | 0.4227 | 0.5773 | Vol. Est. |
| 7.44 | — | — | 280 | — | — | 0.7109 | 0.2891 | No |
| 9.15 | — | — | 280 | — | — | 0.6388 | 0.3612 | No |
| 11.27 | — | — | 280 | — | — | 0.5749 | 0.4251 | No |
| 13.80 | — | — | 280 | 0.8900 | 0.1100 | 0.5269 | 0.4731 | Vol. Est. |
| 18.35 | — | — | 280 | 0.8420 | 0.1580 | 0.4834 | 0.5166 | Vol. Est. |
| 20.30 | — | — | 280 | 0.8209 | 0.1791 | 0.4745 | 0.5255 | Vol. Est. |
| 22.62 | — | — | 280 | 0.8000 | 0.2000 | 0.4736 | 0.5264 | Vol. Est. |
| 24.56 | — | — | 280 | 0.7805 | 0.2195 | — | — | No |
| 26.01 | — | — | 280 | 0.7642 | 0.2358 | 0.4806 | 0.5194 | Vol. Est. |
| 27.45 | — | — | 280 | 0.7464 | 0.2536 | 0.4867 | 0.5133 | Vol. Est. |
| 29.25 | — | — | 280 | 0.7255 | 0.2745 | 0.4961 | 0.5039 | Vol. Est. |
| 31.19 | — | — | 280 | 0.6957 | 0.3043 | 0.5260 | 0.4740 | Vol. Est. |
| 31.96 | — | — | 280 | 0.6730 | 0.3270 | 0.5528 | 0.4472 | Vol. Est. |
| 8.53 | — | — | 290 | 0.9595 | 0.0405 | 0.8012 | 0.1988 | Vol. Est. |
| 9.49 | — | — | 290 | 0.9472 | 0.0528 | 0.7658 | 0.2342 | Vol. Est. |
| 11.29 | — | — | 290 | 0.9196 | 0.0804 | 0.7133 | 0.2867 | Vol. Est. |
| 11.72 | — | — | 290 | — | — | 0.7031 | 0.2969 | No |
| 13.88 | — | — | 290 | 0.8774 | 0.1226 | 0.6704 | 0.3296 | Vol. Est. |
| 15.65 | — | — | 290 | 0.8551 | 0.1449 | 0.6540 | 0.3460 | Vol. Est. |
| 17.27 | — | — | 290 | 0.8330 | 0.1670 | 0.6475 | 0.3525 | Vol. Est. |
| 18.95 | — | — | 290 | 0.8080 | 0.1920 | 0.6673 | 0.3327 | Vol. Est. |
| 19.71 | — | — | 290 | 0.7935 | 0.2065 | 0.6759 | 0.3241 | Vol. Est. |

Continued: Data summarised from Table 1 of Tsang81 [110]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | y_{CO_2} | y_{H_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 6.079500 | — | — | 273.15 | — | — | 0.7170 | 0.2830 | No |
| 10.436475 | — | — | 273.15 | 0.9530 | 0.0470 | 0.5260 | 0.4740 | Vol. Est. |
| 13.881525 | — | — | 273.15 | 0.9211 | 0.0789 | 0.4370 | 0.5630 | Vol. Est. |
| 18.339825 | — | — | 273.15 | 0.8960 | 0.1040 | 0.4040 | 0.5960 | Vol. Est. |
| 23.304750 | — | — | 273.15 | 0.8440 | 0.1560 | 0.3750 | 0.6250 | Vol. Est. |
| 27.763050 | — | — | 273.15 | 0.8200 | 0.1800 | 0.3510 | 0.6490 | Vol. Est. |
| 30.296175 | — | — | 273.15 | 0.7860 | 0.2140 | 0.3490 | 0.6510 | Vol. Est. |
| 31.309425 | — | — | 273.15 | 0.7770 | 0.2230 | — | — | No |
| 34.045200 | — | — | 273.15 | 0.7140 | 0.2860 | 0.3960 | 0.6040 | Vol. Est. |
| 35.463750 | — | — | 273.15 | 0.6830 | 0.3170 | 0.4200 | 0.5800 | Vol. Est. |
| 36.274350 | — | — | 273.15 | 0.6790 | 0.3210 | 0.4660 | 0.5340 | Vol. Est. |
| 37.490250 | — | — | 273.15 | 0.5280 | 0.4720 | 0.5220 | 0.4780 | Vol. Est. |

Data summarised from Table 2 of Yorizane70 [84]

7.1.4 Carbon Dioxide–Hydrogen Density Data

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 5.06625 | 0.00048430 | 323.15 | 0.527 | 0.473 | Yes |
| 10.13250 | 0.00024100 | 323.15 | 0.527 | 0.473 | Yes |
| 20.26500 | 0.00011790 | 323.15 | 0.527 | 0.473 | Yes |
| 30.39750 | 0.00008247 | 323.15 | 0.527 | 0.473 | Yes |
| 40.53000 | 0.00006618 | 323.15 | 0.527 | 0.473 | Yes |
| 50.66250 | 0.00005692 | 323.15 | 0.527 | 0.473 | Yes |
| 5.06625 | 0.00058820 | 373.15 | 0.527 | 0.473 | Yes |
| 10.13250 | 0.00029370 | 373.15 | 0.527 | 0.473 | Yes |
| 20.26500 | 0.00014620 | 373.15 | 0.527 | 0.473 | Yes |
| 30.39750 | 0.00010150 | 373.15 | 0.527 | 0.473 | Yes |
| 40.53000 | 0.00007943 | 373.15 | 0.527 | 0.473 | Yes |
| 50.66250 | 0.00006689 | 373.15 | 0.527 | 0.473 | Yes |
| 5.06625 | 0.00068710 | 423.15 | 0.527 | 0.473 | Yes |
| 10.13250 | 0.00034160 | 423.15 | 0.527 | 0.473 | Yes |
| 20.26500 | 0.00017120 | 423.15 | 0.527 | 0.473 | Yes |
| 30.39750 | 0.00011810 | 423.15 | 0.527 | 0.473 | Yes |
| 40.53000 | 0.00009276 | 423.15 | 0.527 | 0.473 | Yes |
| 50.66250 | 0.00007806 | 423.15 | 0.527 | 0.473 | Yes |
| 5.06625 | 0.00075760 | 473.15 | 0.527 | 0.473 | Yes |
| 10.13250 | 0.00037450 | 473.15 | 0.527 | 0.473 | Yes |
| 20.26500 | 0.00019690 | 473.15 | 0.527 | 0.473 | Yes |
| 30.39750 | 0.00013610 | 473.15 | 0.527 | 0.473 | Yes |
| 40.53000 | 0.00010700 | 473.15 | 0.527 | 0.473 | Yes |
| 50.66250 | 0.00008985 | 473.15 | 0.527 | 0.473 | Yes |
| 5.06625 | 0.00043880 | 273.15 | 0.264 | 0.736 | Yes |
| 10.13250 | 0.00021830 | 273.15 | 0.264 | 0.736 | Yes |
| 20.26500 | 0.00011330 | 273.15 | 0.264 | 0.736 | Yes |
| 30.39750 | 0.00008006 | 273.15 | 0.264 | 0.736 | Yes |
| 40.53000 | 0.00006412 | 273.15 | 0.264 | 0.736 | Yes |
| 50.66250 | 0.00005488 | 273.15 | 0.264 | 0.736 | Yes |
| 5.06625 | 0.00052360 | 323.15 | 0.264 | 0.736 | Yes |
| 10.13250 | 0.00026600 | 323.15 | 0.264 | 0.736 | Yes |
| 20.26500 | 0.00013770 | 323.15 | 0.264 | 0.736 | Yes |
| 30.39750 | 0.00009553 | 323.15 | 0.264 | 0.736 | Yes |
| 40.53000 | 0.00007680 | 323.15 | 0.264 | 0.736 | Yes |
| 50.66250 | 0.00006452 | 323.15 | 0.264 | 0.736 | Yes |
| 5.06625 | 0.00061350 | 373.15 | 0.264 | 0.736 | Yes |
| 10.13250 | 0.00030960 | 373.15 | 0.264 | 0.736 | Yes |
| 20.26500 | 0.00016040 | 373.15 | 0.264 | 0.736 | Yes |
| 30.39750 | 0.00011220 | 373.15 | 0.264 | 0.736 | Yes |
| 40.53000 | 0.00008842 | 373.15 | 0.264 | 0.736 | Yes |
| 50.66250 | 0.00007413 | 373.15 | 0.264 | 0.736 | Yes |
| 5.06625 | 0.00069930 | 423.15 | 0.264 | 0.736 | Yes |
| 10.13250 | 0.00035460 | 423.15 | 0.264 | 0.736 | Yes |
| 20.26500 | 0.00018350 | 423.15 | 0.264 | 0.736 | Yes |
| 30.39750 | 0.00012780 | 423.15 | 0.264 | 0.736 | Yes |
| 40.53000 | 0.00009881 | 423.15 | 0.264 | 0.736 | Yes |
| 50.66250 | 0.00008361 | 423.15 | 0.264 | 0.736 | Yes |
| 5.06625 | 0.00076920 | 473.15 | 0.264 | 0.736 | Yes |
| 10.13250 | 0.00039220 | 473.15 | 0.264 | 0.736 | Yes |
| 20.26500 | 0.00020470 | 473.15 | 0.264 | 0.736 | Yes |
| 30.39750 | 0.00014200 | 473.15 | 0.264 | 0.736 | Yes |
| 40.53000 | 0.00011090 | 473.15 | 0.264 | 0.736 | Yes |
| 50.66250 | 0.00009234 | 473.15 | 0.264 | 0.736 | Yes |

Data summarised from Table 1 of Kritschewsky40 [99]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 0.1000 | 0.026881618 | 323.15 | 0.1367 | 0.8633 | Yes |
| 0.5000 | 0.005386534 | 323.15 | 0.1367 | 0.8633 | Yes |
| 1.0000 | 0.002699984 | 323.15 | 0.1367 | 0.8633 | Yes |
| 1.5000 | 0.001927344 | 323.15 | 0.1367 | 0.8633 | Yes |
| 2.0000 | 0.001357112 | 323.15 | 0.1367 | 0.8633 | Yes |
| 2.5000 | 0.001088591 | 323.15 | 0.1367 | 0.8633 | Yes |
| 3.0000 | 0.000909488 | 323.15 | 0.1367 | 0.8633 | Yes |
| 3.5000 | 0.00078148 | 323.15 | 0.1367 | 0.8633 | Yes |
| 4.0000 | 0.00068534 | 323.15 | 0.1367 | 0.8633 | Yes |
| 4.5000 | 0.000610445 | 323.15 | 0.1367 | 0.8633 | Yes |
| 5.0000 | 0.000550422 | 323.15 | 0.1367 | 0.8633 | Yes |
| 5.5000 | 0.000501116 | 323.15 | 0.1367 | 0.8633 | Yes |
| 6.0000 | 0.000459849 | 323.15 | 0.1367 | 0.8633 | Yes |
| 0.1000 | 0.028961273 | 348.15 | 0.1367 | 0.8633 | Yes |
| 0.5000 | 0.005803254 | 348.15 | 0.1367 | 0.8633 | Yes |
| 1.0000 | 0.002908864 | 348.15 | 0.1367 | 0.8633 | Yes |
| 1.5000 | 0.00194426 | 348.15 | 0.1367 | 0.8633 | Yes |
| 2.0000 | 0.001461958 | 348.15 | 0.1367 | 0.8633 | Yes |
| 2.5000 | 0.001172693 | 348.15 | 0.1367 | 0.8633 | Yes |
| 3.0000 | 0.000979849 | 348.15 | 0.1367 | 0.8633 | Yes |

Data summarised from TABLE 1 of Mallu90 [122]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 3.5000 | 0.000842104 | 348.15 | 0.1367 | 0.8633 | Yes |
| 4.0000 | 0.000738722 | 348.15 | 0.1367 | 0.8633 | Yes |
| 4.5000 | 0.00065825 | 348.15 | 0.1367 | 0.8633 | Yes |
| 5.0000 | 0.000593815 | 348.15 | 0.1367 | 0.8633 | Yes |
| 5.5000 | 0.000540937 | 348.15 | 0.1367 | 0.8633 | Yes |
| 6.0000 | 0.000496824 | 348.15 | 0.1367 | 0.8633 | Yes |
| 0.1000 | 0.031040928 | 373.15 | 0.1367 | 0.8633 | Yes |
| 0.5000 | 0.006219355 | 373.15 | 0.1367 | 0.8633 | Yes |
| 1.0000 | 0.003117434 | 373.15 | 0.1367 | 0.8633 | Yes |
| 1.5000 | 0.002083667 | 373.15 | 0.1367 | 0.8633 | Yes |
| 2.0000 | 0.001566783 | 373.15 | 0.1367 | 0.8633 | Yes |
| 2.5000 | 0.001256902 | 373.15 | 0.1367 | 0.8633 | Yes |
| 3.0000 | 0.00105021 | 373.15 | 0.1367 | 0.8633 | Yes |
| 3.5000 | 0.000902662 | 373.15 | 0.1367 | 0.8633 | Yes |
| 4.0000 | 0.000791924 | 373.15 | 0.1367 | 0.8633 | Yes |
| 4.5000 | 0.000705725 | 373.15 | 0.1367 | 0.8633 | Yes |
| 5.0000 | 0.000636766 | 373.15 | 0.1367 | 0.8633 | Yes |
| 5.5000 | 0.000580288 | 373.15 | 0.1367 | 0.8633 | Yes |
| 6.0000 | 0.00053312 | 373.15 | 0.1367 | 0.8633 | Yes |
| 0.1000 | 0.033120583 | 398.15 | 0.1367 | 0.8633 | Yes |
| 0.5000 | 0.006636034 | 398.15 | 0.1367 | 0.8633 | Yes |
| 1.0000 | 0.003326293 | 398.15 | 0.1367 | 0.8633 | Yes |
| 1.5000 | 0.002223046 | 398.15 | 0.1367 | 0.8633 | Yes |
| 2.0000 | 0.001671754 | 398.15 | 0.1367 | 0.8633 | Yes |
| 2.5000 | 0.001340978 | 398.15 | 0.1367 | 0.8633 | Yes |
| 3.0000 | 0.001120461 | 398.15 | 0.1367 | 0.8633 | Yes |
| 3.5000 | 0.000963044 | 398.15 | 0.1367 | 0.8633 | Yes |
| 4.0000 | 0.000844898 | 398.15 | 0.1367 | 0.8633 | Yes |
| 4.5000 | 0.000753006 | 398.15 | 0.1367 | 0.8633 | Yes |
| 5.0000 | 0.000679427 | 398.15 | 0.1367 | 0.8633 | Yes |
| 5.5000 | 0.000619226 | 398.15 | 0.1367 | 0.8633 | Yes |
| 6.0000 | 0.000568948 | 398.15 | 0.1367 | 0.8633 | Yes |
| 0.1000 | 0.035200238 | 423.15 | 0.1367 | 0.8633 | Yes |
| 0.5000 | 0.007052713 | 423.15 | 0.1367 | 0.8633 | Yes |
| 1.0000 | 0.003535152 | 423.15 | 0.1367 | 0.8633 | Yes |
| 1.5000 | 0.002362632 | 423.15 | 0.1367 | 0.8633 | Yes |
| 2.0000 | 0.001776548 | 423.15 | 0.1367 | 0.8633 | Yes |
| 2.5000 | 0.001425038 | 423.15 | 0.1367 | 0.8633 | Yes |
| 3.0000 | 0.001190698 | 423.15 | 0.1367 | 0.8633 | Yes |
| 3.5000 | 0.001023312 | 423.15 | 0.1367 | 0.8633 | Yes |
| 4.0000 | 0.000897773 | 423.15 | 0.1367 | 0.8633 | Yes |
| 4.5000 | 0.000800053 | 423.15 | 0.1367 | 0.8633 | Yes |
| 5.0000 | 0.000721878 | 423.15 | 0.1367 | 0.8633 | Yes |
| 5.5000 | 0.000657788 | 423.15 | 0.1367 | 0.8633 | Yes |
| 6.0000 | 0.000604321 | 423.15 | 0.1367 | 0.8633 | Yes |
| 0.1000 | 0.026814448 | 323.15 | 0.7659 | 0.2341 | Yes |
| 0.5000 | 0.005319363 | 323.15 | 0.7659 | 0.2341 | Yes |
| 1.0000 | 0.002632545 | 323.15 | 0.7659 | 0.2341 | Yes |
| 1.5000 | 0.001736939 | 323.15 | 0.7659 | 0.2341 | Yes |
| 2.0000 | 0.001289135 | 323.15 | 0.7659 | 0.2341 | Yes |
| 2.5000 | 0.001020561 | 323.15 | 0.7659 | 0.2341 | Yes |
| 3.0000 | 0.000841422 | 323.15 | 0.7659 | 0.2341 | Yes |
| 3.5000 | 0.000713542 | 323.15 | 0.7659 | 0.2341 | Yes |
| 4.0000 | 0.000617565 | 323.15 | 0.7659 | 0.2341 | Yes |
| 4.5000 | 0.000542916 | 323.15 | 0.7659 | 0.2341 | Yes |
| 5.0000 | 0.000483197 | 323.15 | 0.7659 | 0.2341 | Yes |
| 5.5000 | 0.000434385 | 323.15 | 0.7659 | 0.2341 | Yes |
| 6.0000 | 0.000393708 | 323.15 | 0.7659 | 0.2341 | Yes |
| 0.1000 | 0.02890338 | 348.15 | 0.7659 | 0.2341 | Yes |
| 0.5000 | 0.005744782 | 348.15 | 0.7659 | 0.2341 | Yes |
| 1.0000 | 0.002850391 | 348.15 | 0.7659 | 0.2341 | Yes |
| 1.5000 | 0.001885788 | 348.15 | 0.7659 | 0.2341 | Yes |
| 2.0000 | 0.001403486 | 348.15 | 0.7659 | 0.2341 | Yes |
| 2.5000 | 0.00111422 | 348.15 | 0.7659 | 0.2341 | Yes |
| 3.0000 | 0.000921473 | 348.15 | 0.7659 | 0.2341 | Yes |
| 3.5000 | 0.000783797 | 348.15 | 0.7659 | 0.2341 | Yes |
| 4.0000 | 0.000680612 | 348.15 | 0.7659 | 0.2341 | Yes |
| 4.5000 | 0.000600357 | 348.15 | 0.7659 | 0.2341 | Yes |
| 5.0000 | 0.000536153 | 348.15 | 0.7659 | 0.2341 | Yes |
| 5.5000 | 0.000483622 | 348.15 | 0.7659 | 0.2341 | Yes |
| 6.0000 | 0.000439895 | 348.15 | 0.7659 | 0.2341 | Yes |
| 0.1000 | 0.030988185 | 373.15 | 0.7659 | 0.2341 | Yes |
| 0.5000 | 0.006169094 | 373.15 | 0.7659 | 0.2341 | Yes |
| 1.0000 | 0.003066862 | 373.15 | 0.7659 | 0.2341 | Yes |
| 1.5000 | 0.002032992 | 373.15 | 0.7659 | 0.2341 | Yes |
| 2.0000 | 0.001516212 | 373.15 | 0.7659 | 0.2341 | Yes |
| 2.5000 | 0.001206268 | 373.15 | 0.7659 | 0.2341 | Yes |
| 3.0000 | 0.000999639 | 373.15 | 0.7659 | 0.2341 | Yes |
| 3.5000 | 0.000852224 | 373.15 | 0.7659 | 0.2341 | Yes |
| 4.0000 | 0.000741663 | 373.15 | 0.7659 | 0.2341 | Yes |
| 4.5000 | 0.00065567 | 373.15 | 0.7659 | 0.2341 | Yes |
| 5.0000 | 0.000586939 | 373.15 | 0.7659 | 0.2341 | Yes |
| 5.5000 | 0.000530704 | 373.15 | 0.7659 | 0.2341 | Yes |
| 6.0000 | 0.000483893 | 373.15 | 0.7659 | 0.2341 | Yes |

Continued: Data summarised from TABLE 1 of Mallu90 [122]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 0.1000 | 0.033074237 | 398.15 | 0.7659 | 0.2341 | Yes |
| 0.5000 | 0.006592337 | 398.15 | 0.7659 | 0.2341 | Yes |
| 1.0000 | 0.003282265 | 398.15 | 0.7659 | 0.2341 | Yes |
| 1.5000 | 0.002178907 | 398.15 | 0.7659 | 0.2341 | Yes |
| 2.0000 | 0.00162756 | 398.15 | 0.7659 | 0.2341 | Yes |
| 2.5000 | 0.001296884 | 398.15 | 0.7659 | 0.2341 | Yes |
| 3.0000 | 0.001076433 | 398.15 | 0.7659 | 0.2341 | Yes |
| 3.5000 | 0.000919062 | 398.15 | 0.7659 | 0.2341 | Yes |
| 4.0000 | 0.000801035 | 398.15 | 0.7659 | 0.2341 | Yes |
| 4.5000 | 0.000709309 | 398.15 | 0.7659 | 0.2341 | Yes |
| 5.0000 | 0.000635995 | 398.15 | 0.7659 | 0.2341 | Yes |
| 5.5000 | 0.00057601 | 398.15 | 0.7659 | 0.2341 | Yes |
| 6.0000 | 0.000526078 | 398.15 | 0.7659 | 0.2341 | Yes |
| 0.1000 | 0.035161537 | 423.15 | 0.7659 | 0.2341 | Yes |
| 0.5000 | 0.007014716 | 423.15 | 0.7659 | 0.2341 | Yes |
| 1.0000 | 0.003496451 | 423.15 | 0.7659 | 0.2341 | Yes |
| 1.5000 | 0.002324166 | 423.15 | 0.7659 | 0.2341 | Yes |
| 2.0000 | 0.001737847 | 423.15 | 0.7659 | 0.2341 | Yes |
| 2.5000 | 0.001386337 | 423.15 | 0.7659 | 0.2341 | Yes |
| 3.0000 | 0.001151997 | 423.15 | 0.7659 | 0.2341 | Yes |
| 3.5000 | 0.000984611 | 423.15 | 0.7659 | 0.2341 | Yes |
| 4.0000 | 0.00085916 | 423.15 | 0.7659 | 0.2341 | Yes |
| 4.5000 | 0.000761587 | 423.15 | 0.7659 | 0.2341 | Yes |
| 5.0000 | 0.000683669 | 423.15 | 0.7659 | 0.2341 | Yes |
| 5.5000 | 0.000619854 | 423.15 | 0.7659 | 0.2341 | Yes |
| 6.0000 | 0.000566734 | 423.15 | 0.7659 | 0.2341 | Yes |

Continued: Data summarised from TABLE 1 of Mallu90 [122]

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 19.80 | 0.0000498164 | 288.15 | 0.9003 | 0.0997 | Yes |
| 18.56 | 0.0000506270 | 288.15 | 0.9003 | 0.0997 | Yes |
| 17.45 | 0.0000514578 | 288.15 | 0.9003 | 0.0997 | Yes |
| 16.52 | 0.0000522820 | 288.15 | 0.9003 | 0.0997 | Yes |
| 15.74 | 0.0000530764 | 288.15 | 0.9003 | 0.0997 | Yes |
| 15.06 | 0.0000538588 | 288.15 | 0.9003 | 0.0997 | Yes |
| 14.53 | 0.0000545748 | 288.15 | 0.9003 | 0.0997 | Yes |
| 20.75 | 0.0000480527 | 288.15 | 0.9252 | 0.0748 | Yes |
| 19.35 | 0.0000486940 | 288.15 | 0.9252 | 0.0748 | Yes |
| 17.88 | 0.0000494242 | 288.15 | 0.9252 | 0.0748 | Yes |
| 17.65 | 0.0000495560 | 288.15 | 0.9252 | 0.0748 | Yes |
| 16.46 | 0.0000502816 | 288.15 | 0.9252 | 0.0748 | Yes |
| 15.49 | 0.0000509650 | 288.15 | 0.9252 | 0.0748 | Yes |
| 14.56 | 0.0000517262 | 288.15 | 0.9252 | 0.0748 | Yes |
| 13.79 | 0.0000524700 | 288.15 | 0.9252 | 0.0748 | Yes |
| 13.14 | 0.0000531731 | 288.15 | 0.9252 | 0.0748 | Yes |
| 12.60 | 0.0000538386 | 288.15 | 0.9252 | 0.0748 | Yes |
| 22.26 | 0.0000457929 | 288.15 | 0.9803 | 0.0197 | Yes |
| 20.08 | 0.0000463782 | 288.15 | 0.9803 | 0.0197 | Yes |
| 18.21 | 0.0000469377 | 288.15 | 0.9803 | 0.0197 | Yes |
| 16.55 | 0.0000475057 | 288.15 | 0.9803 | 0.0197 | Yes |
| 15.07 | 0.0000480716 | 288.15 | 0.9803 | 0.0197 | Yes |
| 13.75 | 0.0000486456 | 288.15 | 0.9803 | 0.0197 | Yes |
| 12.59 | 0.0000492167 | 288.15 | 0.9803 | 0.0197 | Yes |
| 11.58 | 0.0000497783 | 288.15 | 0.9803 | 0.0197 | Yes |
| 10.70 | 0.0000503354 | 288.15 | 0.9803 | 0.0197 | Yes |
| 9.93 | 0.0000508870 | 288.15 | 0.9803 | 0.0197 | Yes |
| 9.27 | 0.0000514264 | 288.15 | 0.9803 | 0.0197 | Yes |
| 8.69 | 0.0000519523 | 288.15 | 0.9803 | 0.0197 | Yes |
| 8.20 | 0.0000524508 | 288.15 | 0.9803 | 0.0197 | Yes |
| 7.77 | 0.0000529395 | 288.15 | 0.9803 | 0.0197 | Yes |
| 19.16 | 0.0000521081 | 293.15 | 0.9000 | 0.1000 | Yes |
| 18.24 | 0.0000528904 | 293.15 | 0.9000 | 0.1000 | Yes |
| 17.47 | 0.0000536459 | 293.15 | 0.9000 | 0.1000 | Yes |
| 16.78 | 0.0000544009 | 293.15 | 0.9000 | 0.1000 | Yes |
| 16.17 | 0.0000551546 | 293.15 | 0.9000 | 0.1000 | Yes |
| 15.63 | 0.0000559138 | 293.15 | 0.9000 | 0.1000 | Yes |
| 15.15 | 0.0000566699 | 293.15 | 0.9000 | 0.1000 | Yes |
| 14.72 | 0.0000574302 | 293.15 | 0.9000 | 0.1000 | Yes |
| 14.33 | 0.0000581856 | 293.15 | 0.9000 | 0.1000 | Yes |
| 14.00 | 0.0000589263 | 293.15 | 0.9000 | 0.1000 | Yes |
| 21.72 | 0.0000490707 | 293.15 | 0.9249 | 0.0751 | Yes |
| 20.31 | 0.0000497883 | 293.15 | 0.9249 | 0.0751 | Yes |
| 19.13 | 0.0000504710 | 293.15 | 0.9249 | 0.0751 | Yes |
| 19.08 | 0.0000504959 | 293.15 | 0.9249 | 0.0751 | Yes |
| 18.06 | 0.0000511662 | 293.15 | 0.9249 | 0.0751 | Yes |
| 17.11 | 0.0000518744 | 293.15 | 0.9249 | 0.0751 | Yes |
| 16.27 | 0.0000525753 | 293.15 | 0.9249 | 0.0751 | Yes |
| 15.30 | 0.0000535258 | 293.15 | 0.9249 | 0.0751 | Yes |
| 15.03 | 0.0000538220 | 293.15 | 0.9249 | 0.0751 | Yes |
| 14.20 | 0.0000548332 | 293.15 | 0.9249 | 0.0751 | Yes |
| 13.48 | 0.0000558680 | 293.15 | 0.9249 | 0.0751 | Yes |
| 12.85 | 0.0000569504 | 293.15 | 0.9249 | 0.0751 | Yes |
| 12.69 | 0.0000572698 | 293.15 | 0.9249 | 0.0751 | Yes |

Data summarised from Table S1 of Sanchez–Vicente13 [111]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 22.71 | 0.0000467417 | 293.15 | 0.9799 | 0.0201 | Yes |
| 20.78 | 0.0000473207 | 293.15 | 0.9799 | 0.0201 | Yes |
| 19.09 | 0.0000479036 | 293.15 | 0.9799 | 0.0201 | Yes |
| 17.56 | 0.0000484847 | 293.15 | 0.9799 | 0.0201 | Yes |
| 16.21 | 0.0000490689 | 293.15 | 0.9799 | 0.0201 | Yes |
| 15.00 | 0.0000496502 | 293.15 | 0.9799 | 0.0201 | Yes |
| 13.91 | 0.0000502455 | 293.15 | 0.9799 | 0.0201 | Yes |
| 12.93 | 0.0000508492 | 293.15 | 0.9799 | 0.0201 | Yes |
| 12.06 | 0.0000514615 | 293.15 | 0.9799 | 0.0201 | Yes |
| 11.31 | 0.0000520636 | 293.15 | 0.9799 | 0.0201 | Yes |
| 10.39 | 0.0000529513 | 293.15 | 0.9799 | 0.0201 | Yes |
| 9.78 | 0.0000536156 | 293.15 | 0.9799 | 0.0201 | Yes |
| 9.23 | 0.0000543173 | 293.15 | 0.9799 | 0.0201 | Yes |
| 8.75 | 0.0000550305 | 293.15 | 0.9799 | 0.0201 | Yes |
| 8.07 | 0.0000562496 | 293.15 | 0.9799 | 0.0201 | Yes |
| 22.07 | 0.0000536314 | 303.15 | 0.9000 | 0.1000 | Yes |
| 20.96 | 0.0000546249 | 303.15 | 0.9000 | 0.1000 | Yes |
| 20.02 | 0.0000555859 | 303.15 | 0.9000 | 0.1000 | Yes |
| 19.18 | 0.0000565893 | 303.15 | 0.9000 | 0.1000 | Yes |
| 18.39 | 0.0000576631 | 303.15 | 0.9000 | 0.1000 | Yes |
| 17.74 | 0.0000586399 | 303.15 | 0.9000 | 0.1000 | Yes |
| 17.72 | 0.0000586917 | 303.15 | 0.9000 | 0.1000 | Yes |
| 17.14 | 0.0000596950 | 303.15 | 0.9000 | 0.1000 | Yes |
| 16.57 | 0.0000608632 | 303.15 | 0.9000 | 0.1000 | Yes |
| 16.08 | 0.0000619717 | 303.15 | 0.9000 | 0.1000 | Yes |
| 15.62 | 0.0000631614 | 303.15 | 0.9000 | 0.1000 | Yes |
| 15.22 | 0.0000643456 | 303.15 | 0.9000 | 0.1000 | Yes |
| 14.85 | 0.0000655426 | 303.15 | 0.9000 | 0.1000 | Yes |
| 14.51 | 0.0000667739 | 303.15 | 0.9000 | 0.1000 | Yes |
| 14.21 | 0.0000680407 | 303.15 | 0.9000 | 0.1000 | Yes |
| 13.92 | 0.0000693685 | 303.15 | 0.9000 | 0.1000 | Yes |
| 13.65 | 0.0000707115 | 303.15 | 0.9000 | 0.1000 | Yes |
| 13.01 | 0.0000746355 | 303.15 | 0.9000 | 0.1000 | Yes |
| 12.41 | 0.0000797169 | 303.15 | 0.9000 | 0.1000 | Yes |
| 11.85 | 0.0000855590 | 303.15 | 0.9000 | 0.1000 | Yes |
| 11.30 | 0.0000936279 | 303.15 | 0.9000 | 0.1000 | Yes |
| 10.75 | 0.0001066165 | 303.15 | 0.9000 | 0.1000 | Yes |
| 10.20 | 0.0001204192 | 303.15 | 0.9000 | 0.1000 | Yes |
| 9.66 | 0.0001361512 | 303.15 | 0.9000 | 0.1000 | Yes |
| 9.12 | 0.0001541851 | 303.15 | 0.9000 | 0.1000 | Yes |
| 8.57 | 0.0001752999 | 303.15 | 0.9000 | 0.1000 | Yes |
| 8.04 | 0.0001976693 | 303.15 | 0.9000 | 0.1000 | Yes |
| 7.52 | 0.0002224056 | 303.15 | 0.9000 | 0.1000 | Yes |
| 7.03 | 0.0002486608 | 303.15 | 0.9000 | 0.1000 | Yes |
| 6.61 | 0.0002741777 | 303.15 | 0.9000 | 0.1000 | Yes |
| 5.94 | 0.0003205362 | 303.15 | 0.9000 | 0.1000 | Yes |
| 5.41 | 0.0003655702 | 303.15 | 0.9000 | 0.1000 | Yes |
| 4.87 | 0.0004203865 | 303.15 | 0.9000 | 0.1000 | Yes |
| 4.33 | 0.0004872778 | 303.15 | 0.9000 | 0.1000 | Yes |
| 3.81 | 0.0005711707 | 303.15 | 0.9000 | 0.1000 | Yes |
| 3.28 | 0.0006805231 | 303.15 | 0.9000 | 0.1000 | Yes |
| 2.80 | 0.0008191481 | 303.15 | 0.9000 | 0.1000 | Yes |
| 2.29 | 0.0010286977 | 303.15 | 0.9000 | 0.1000 | Yes |
| 1.78 | 0.0013495119 | 303.15 | 0.9000 | 0.1000 | Yes |
| 22.17 | 0.0000519573 | 303.15 | 0.9246 | 0.0754 | Yes |
| 20.81 | 0.0000529131 | 303.15 | 0.9246 | 0.0754 | Yes |
| 19.67 | 0.0000538337 | 303.15 | 0.9246 | 0.0754 | Yes |
| 18.68 | 0.0000547722 | 303.15 | 0.9246 | 0.0754 | Yes |
| 17.81 | 0.0000557060 | 303.15 | 0.9246 | 0.0754 | Yes |
| 17.04 | 0.0000566565 | 303.15 | 0.9246 | 0.0754 | Yes |
| 16.36 | 0.0000576237 | 303.15 | 0.9246 | 0.0754 | Yes |
| 15.76 | 0.0000586076 | 303.15 | 0.9246 | 0.0754 | Yes |
| 15.20 | 0.0000596693 | 303.15 | 0.9246 | 0.0754 | Yes |
| 14.72 | 0.0000606799 | 303.15 | 0.9246 | 0.0754 | Yes |
| 14.30 | 0.0000617253 | 303.15 | 0.9246 | 0.0754 | Yes |
| 13.92 | 0.0000627881 | 303.15 | 0.9246 | 0.0754 | Yes |
| 13.57 | 0.0000638581 | 303.15 | 0.9246 | 0.0754 | Yes |
| 13.27 | 0.0000649446 | 303.15 | 0.9246 | 0.0754 | Yes |
| 12.99 | 0.0000660794 | 303.15 | 0.9246 | 0.0754 | Yes |
| 12.73 | 0.0000672434 | 303.15 | 0.9246 | 0.0754 | Yes |
| 12.11 | 0.0000709831 | 303.15 | 0.9246 | 0.0754 | Yes |
| 11.52 | 0.0000759882 | 303.15 | 0.9246 | 0.0754 | Yes |
| 10.97 | 0.0000828136 | 303.15 | 0.9246 | 0.0754 | Yes |
| 10.42 | 0.0000920109 | 303.15 | 0.9246 | 0.0754 | Yes |
| 9.92 | 0.0001079663 | 303.15 | 0.9246 | 0.0754 | Yes |
| 9.41 | 0.0001246754 | 303.15 | 0.9246 | 0.0754 | Yes |
| 8.89 | 0.0001450929 | 303.15 | 0.9246 | 0.0754 | Yes |
| 8.37 | 0.0001673920 | 303.15 | 0.9246 | 0.0754 | Yes |
| 7.85 | 0.0001916643 | 303.15 | 0.9246 | 0.0754 | Yes |
| 7.36 | 0.0002174848 | 303.15 | 0.9246 | 0.0754 | Yes |
| 6.91 | 0.0002434067 | 303.15 | 0.9246 | 0.0754 | Yes |
| 6.45 | 0.0002733846 | 303.15 | 0.9246 | 0.0754 | Yes |
| 5.87 | 0.0003156387 | 303.15 | 0.9246 | 0.0754 | Yes |
| 5.33 | 0.0003620891 | 303.15 | 0.9246 | 0.0754 | Yes |
| 4.81 | 0.0004171977 | 303.15 | 0.9246 | 0.0754 | Yes |
| 4.28 | 0.0004856558 | 303.15 | 0.9246 | 0.0754 | Yes |
| 3.75 | 0.0005720399 | 303.15 | 0.9246 | 0.0754 | Yes |
| 3.25 | 0.0006807275 | 303.15 | 0.9246 | 0.0754 | Yes |
| 2.73 | 0.0008335439 | 303.15 | 0.9246 | 0.0754 | Yes |
| 2.22 | 0.0010526715 | 303.15 | 0.9246 | 0.0754 | Yes |
| 1.71 | 0.0013987552 | 303.15 | 0.9246 | 0.0754 | Yes |

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 22.73 | 0.0000490928 | 303.15 | 0.9797 | 0.0203 | Yes |
| 20.81 | 0.0000498931 | 303.15 | 0.9797 | 0.0203 | Yes |
| 19.17 | 0.0000506901 | 303.15 | 0.9797 | 0.0203 | Yes |
| 17.75 | 0.0000514761 | 303.15 | 0.9797 | 0.0203 | Yes |
| 16.55 | 0.0000522488 | 303.15 | 0.9797 | 0.0203 | Yes |
| 15.50 | 0.0000530256 | 303.15 | 0.9797 | 0.0203 | Yes |
| 14.60 | 0.0000537922 | 303.15 | 0.9797 | 0.0203 | Yes |
| 13.82 | 0.0000545469 | 303.15 | 0.9797 | 0.0203 | Yes |
| 13.14 | 0.0000553018 | 303.15 | 0.9797 | 0.0203 | Yes |
| 12.55 | 0.0000560560 | 303.15 | 0.9797 | 0.0203 | Yes |
| 12.04 | 0.0000568012 | 303.15 | 0.9797 | 0.0203 | Yes |
| 11.59 | 0.0000575894 | 303.15 | 0.9797 | 0.0203 | Yes |
| 11.21 | 0.0000583446 | 303.15 | 0.9797 | 0.0203 | Yes |
| 10.87 | 0.0000590875 | 303.15 | 0.9797 | 0.0203 | Yes |
| 10.60 | 0.0000597667 | 303.15 | 0.9797 | 0.0203 | Yes |
| 10.34 | 0.0000604871 | 303.15 | 0.9797 | 0.0203 | Yes |
| 9.77 | 0.0000625200 | 303.15 | 0.9797 | 0.0203 | Yes |
| 9.25 | 0.0000652518 | 303.15 | 0.9797 | 0.0203 | Yes |
| 8.76 | 0.0000692626 | 303.15 | 0.9797 | 0.0203 | Yes |
| 6.24 | 0.0002510618 | 303.15 | 0.9797 | 0.0203 | Yes |
| 6.18 | 0.0002559758 | 303.15 | 0.9797 | 0.0203 | Yes |
| 5.64 | 0.0003011690 | 303.15 | 0.9797 | 0.0203 | Yes |
| 5.10 | 0.0003537502 | 303.15 | 0.9797 | 0.0203 | Yes |
| 4.57 | 0.0004169809 | 303.15 | 0.9797 | 0.0203 | Yes |
| 4.03 | 0.0004943588 | 303.15 | 0.9797 | 0.0203 | Yes |
| 3.50 | 0.0005928231 | 303.15 | 0.9797 | 0.0203 | Yes |
| 2.99 | 0.0007192920 | 303.15 | 0.9797 | 0.0203 | Yes |
| 2.48 | 0.0008991150 | 303.15 | 0.9797 | 0.0203 | Yes |
| 1.97 | 0.0011664195 | 303.15 | 0.9797 | 0.0203 | Yes |
| 21.75 | 0.0000582793 | 313.15 | 0.9000 | 0.1000 | Yes |
| 20.73 | 0.0000596235 | 313.15 | 0.9000 | 0.1000 | Yes |
| 19.84 | 0.0000609844 | 313.15 | 0.9000 | 0.1000 | Yes |
| 19.04 | 0.0000623893 | 313.15 | 0.9000 | 0.1000 | Yes |
| 18.33 | 0.0000638195 | 313.15 | 0.9000 | 0.1000 | Yes |
| 17.68 | 0.0000652954 | 313.15 | 0.9000 | 0.1000 | Yes |
| 17.11 | 0.0000667963 | 313.15 | 0.9000 | 0.1000 | Yes |
| 16.60 | 0.0000683326 | 313.15 | 0.9000 | 0.1000 | Yes |
| 16.14 | 0.0000698677 | 313.15 | 0.9000 | 0.1000 | Yes |
| 15.72 | 0.0000714732 | 313.15 | 0.9000 | 0.1000 | Yes |
| 15.32 | 0.0000730604 | 313.15 | 0.9000 | 0.1000 | Yes |
| 14.96 | 0.0000747898 | 313.15 | 0.9000 | 0.1000 | Yes |
| 14.64 | 0.0000764559 | 313.15 | 0.9000 | 0.1000 | Yes |
| 14.34 | 0.0000781826 | 313.15 | 0.9000 | 0.1000 | Yes |
| 14.06 | 0.0000799249 | 313.15 | 0.9000 | 0.1000 | Yes |
| 13.41 | 0.0000847756 | 313.15 | 0.9000 | 0.1000 | Yes |
| 12.79 | 0.0000904992 | 313.15 | 0.9000 | 0.1000 | Yes |
| 12.20 | 0.0000975272 | 313.15 | 0.9000 | 0.1000 | Yes |
| 11.62 | 0.0001062466 | 313.15 | 0.9000 | 0.1000 | Yes |
| 11.08 | 0.0001162353 | 313.15 | 0.9000 | 0.1000 | Yes |
| 10.53 | 0.0001293392 | 313.15 | 0.9000 | 0.1000 | Yes |
| 9.98 | 0.0001436687 | 313.15 | 0.9000 | 0.1000 | Yes |
| 9.43 | 0.0001602681 | 313.15 | 0.9000 | 0.1000 | Yes |
| 8.88 | 0.0001807108 | 313.15 | 0.9000 | 0.1000 | Yes |
| 8.34 | 0.0002017770 | 313.15 | 0.9000 | 0.1000 | Yes |
| 7.81 | 0.0002261966 | 313.15 | 0.9000 | 0.1000 | Yes |
| 7.30 | 0.0002518065 | 313.15 | 0.9000 | 0.1000 | Yes |
| 6.81 | 0.0002787857 | 313.15 | 0.9000 | 0.1000 | Yes |
| 6.37 | 0.0003060000 | 313.15 | 0.9000 | 0.1000 | Yes |
| 5.73 | 0.0003541868 | 313.15 | 0.9000 | 0.1000 | Yes |
| 5.19 | 0.0004029413 | 313.15 | 0.9000 | 0.1000 | Yes |
| 4.65 | 0.0004623763 | 313.15 | 0.9000 | 0.1000 | Yes |
| 4.12 | 0.0005365310 | 313.15 | 0.9000 | 0.1000 | Yes |
| 3.59 | 0.0006309128 | 313.15 | 0.9000 | 0.1000 | Yes |
| 3.08 | 0.0007539886 | 313.15 | 0.9000 | 0.1000 | Yes |
| 2.56 | 0.0009279860 | 313.15 | 0.9000 | 0.1000 | Yes |
| 2.05 | 0.0011848393 | 313.15 | 0.9000 | 0.1000 | Yes |
| 1.55 | 0.0015988193 | 313.15 | 0.9000 | 0.1000 | Yes |
| 21.49 | 0.0000563769 | 313.15 | 0.9245 | 0.0755 | Yes |
| 20.35 | 0.0000576340 | 313.15 | 0.9245 | 0.0755 | Yes |
| 19.35 | 0.0000589144 | 313.15 | 0.9245 | 0.0755 | Yes |
| 18.49 | 0.0000602085 | 313.15 | 0.9245 | 0.0755 | Yes |
| 17.70 | 0.0000615608 | 313.15 | 0.9245 | 0.0755 | Yes |
| 17.01 | 0.0000629461 | 313.15 | 0.9245 | 0.0755 | Yes |
| 16.41 | 0.0000643648 | 313.15 | 0.9245 | 0.0755 | Yes |
| 15.88 | 0.0000657640 | 313.15 | 0.9245 | 0.0755 | Yes |
| 15.40 | 0.0000672476 | 313.15 | 0.9245 | 0.0755 | Yes |
| 14.96 | 0.0000687880 | 313.15 | 0.9245 | 0.0755 | Yes |
| 14.56 | 0.0000703886 | 313.15 | 0.9245 | 0.0755 | Yes |
| 14.20 | 0.0000719384 | 313.15 | 0.9245 | 0.0755 | Yes |
| 13.87 | 0.0000736377 | 313.15 | 0.9245 | 0.0755 | Yes |
| 13.57 | 0.0000752940 | 313.15 | 0.9245 | 0.0755 | Yes |
| 13.30 | 0.0000770410 | 313.15 | 0.9245 | 0.0755 | Yes |
| 12.64 | 0.0000820564 | 313.15 | 0.9245 | 0.0755 | Yes |
| 12.03 | 0.0000883971 | 313.15 | 0.9245 | 0.0755 | Yes |
| 10.89 | 0.0001063804 | 313.15 | 0.9245 | 0.0755 | Yes |
| 10.34 | 0.0001203284 | 313.15 | 0.9245 | 0.0755 | Yes |
| 9.84 | 0.0001341197 | 313.15 | 0.9245 | 0.0755 | Yes |
| 9.32 | 0.0001511453 | 313.15 | 0.9245 | 0.0755 | Yes |
| 8.79 | 0.0001705196 | 313.15 | 0.9245 | 0.0755 | Yes |

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 8.27 | 0.0001941962 | 313.15 | 0.9245 | 0.0755 | Yes |
| 7.75 | 0.0002181595 | 313.15 | 0.9245 | 0.0755 | Yes |
| 7.27 | 0.0002430920 | 313.15 | 0.9245 | 0.0755 | Yes |
| 6.83 | 0.0002681514 | 313.15 | 0.9245 | 0.0755 | Yes |
| 6.22 | 0.0003079898 | 313.15 | 0.9245 | 0.0755 | Yes |
| 5.70 | 0.0003487571 | 313.15 | 0.9245 | 0.0755 | Yes |
| 5.16 | 0.0003980454 | 313.15 | 0.9245 | 0.0755 | Yes |
| 4.63 | 0.0004578414 | 313.15 | 0.9245 | 0.0755 | Yes |
| 4.10 | 0.0005324570 | 313.15 | 0.9245 | 0.0755 | Yes |
| 3.58 | 0.0006282993 | 313.15 | 0.9245 | 0.0755 | Yes |
| 3.06 | 0.0007534954 | 313.15 | 0.9245 | 0.0755 | Yes |
| 2.55 | 0.0009281694 | 313.15 | 0.9245 | 0.0755 | Yes |
| 2.06 | 0.0011769295 | 313.15 | 0.9245 | 0.0755 | Yes |
| 1.56 | 0.0015890838 | 313.15 | 0.9245 | 0.0755 | Yes |
| 21.17 | 0.0000528373 | 313.15 | 0.9797 | 0.0203 | Yes |
| 19.18 | 0.0000542180 | 313.15 | 0.9797 | 0.0203 | Yes |
| 17.49 | 0.0000556871 | 313.15 | 0.9797 | 0.0203 | Yes |
| 15.74 | 0.0000577204 | 313.15 | 0.9797 | 0.0203 | Yes |
| 15.40 | 0.0000581951 | 313.15 | 0.9797 | 0.0203 | Yes |
| 13.88 | 0.0000608367 | 313.15 | 0.9797 | 0.0203 | Yes |
| 13.65 | 0.0000613381 | 313.15 | 0.9797 | 0.0203 | Yes |
| 12.62 | 0.0000640795 | 313.15 | 0.9797 | 0.0203 | Yes |
| 11.77 | 0.0000673915 | 313.15 | 0.9797 | 0.0203 | Yes |
| 11.56 | 0.0000683954 | 313.15 | 0.9797 | 0.0203 | Yes |
| 10.81 | 0.0000735472 | 313.15 | 0.9797 | 0.0203 | Yes |
| 10.24 | 0.0000801291 | 313.15 | 0.9797 | 0.0203 | Yes |
| 9.74 | 0.0000900616 | 313.15 | 0.9797 | 0.0203 | Yes |
| 9.35 | 0.0001028540 | 313.15 | 0.9797 | 0.0203 | Yes |
| 8.99 | 0.0001198820 | 313.15 | 0.9797 | 0.0203 | Yes |
| 8.62 | 0.0001405325 | 313.15 | 0.9797 | 0.0203 | Yes |
| 8.36 | 0.0001536402 | 313.15 | 0.9797 | 0.0203 | Yes |
| 8.26 | 0.0001594883 | 313.15 | 0.9797 | 0.0203 | Yes |
| 7.65 | 0.0001943157 | 313.15 | 0.9797 | 0.0203 | Yes |
| 6.83 | 0.0002442418 | 313.15 | 0.9797 | 0.0203 | Yes |
| 6.35 | 0.0002771838 | 313.15 | 0.9797 | 0.0203 | Yes |
| 5.82 | 0.0003180363 | 313.15 | 0.9797 | 0.0203 | Yes |
| 5.32 | 0.0003626683 | 313.15 | 0.9797 | 0.0203 | Yes |
| 4.81 | 0.0004181930 | 313.15 | 0.9797 | 0.0203 | Yes |
| 4.29 | 0.0004865561 | 313.15 | 0.9797 | 0.0203 | Yes |
| 3.77 | 0.0005723809 | 313.15 | 0.9797 | 0.0203 | Yes |
| 3.26 | 0.0006839544 | 313.15 | 0.9797 | 0.0203 | Yes |
| 2.75 | 0.0008363861 | 313.15 | 0.9797 | 0.0203 | Yes |
| 2.24 | 0.0010526225 | 313.15 | 0.9797 | 0.0203 | Yes |
| 1.75 | 0.0013877017 | 313.15 | 0.9797 | 0.0203 | Yes |
| 20.23 | 0.0000664437 | 323.15 | 0.8999 | 0.1001 | Yes |
| 19.07 | 0.0000691924 | 323.15 | 0.8999 | 0.1001 | Yes |
| 18.08 | 0.0000721784 | 323.15 | 0.8999 | 0.1001 | Yes |
| 17.22 | 0.0000752484 | 323.15 | 0.8999 | 0.1001 | Yes |
| 17.21 | 0.0000752911 | 323.15 | 0.8999 | 0.1001 | Yes |
| 16.45 | 0.0000786222 | 323.15 | 0.8999 | 0.1001 | Yes |
| 15.84 | 0.0000818052 | 323.15 | 0.8999 | 0.1001 | Yes |
| 15.23 | 0.0000854581 | 323.15 | 0.8999 | 0.1001 | Yes |
| 14.78 | 0.0000887150 | 323.15 | 0.8999 | 0.1001 | Yes |
| 14.34 | 0.0000921444 | 323.15 | 0.8999 | 0.1001 | Yes |
| 14.00 | 0.0000951851 | 323.15 | 0.8999 | 0.1001 | Yes |
| 13.66 | 0.0000986039 | 323.15 | 0.8999 | 0.1001 | Yes |
| 13.39 | 0.0001016507 | 323.15 | 0.8999 | 0.1001 | Yes |
| 13.13 | 0.0001048365 | 323.15 | 0.8999 | 0.1001 | Yes |
| 12.42 | 0.0001149809 | 323.15 | 0.8999 | 0.1001 | Yes |
| 11.79 | 0.0001250594 | 323.15 | 0.8999 | 0.1001 | Yes |
| 11.17 | 0.0001368858 | 323.15 | 0.8999 | 0.1001 | Yes |
| 10.51 | 0.0001518749 | 323.15 | 0.8999 | 0.1001 | Yes |
| 9.96 | 0.0001665540 | 323.15 | 0.8999 | 0.1001 | Yes |
| 9.38 | 0.0001842889 | 323.15 | 0.8999 | 0.1001 | Yes |
| 8.82 | 0.0002037175 | 323.15 | 0.8999 | 0.1001 | Yes |
| 8.29 | 0.0002247679 | 323.15 | 0.8999 | 0.1001 | Yes |
| 7.76 | 0.0002487900 | 323.15 | 0.8999 | 0.1001 | Yes |
| 7.24 | 0.0002754768 | 323.15 | 0.8999 | 0.1001 | Yes |
| 6.76 | 0.0003036339 | 323.15 | 0.8999 | 0.1001 | Yes |
| 6.29 | 0.0003347889 | 323.15 | 0.8999 | 0.1001 | Yes |
| 5.77 | 0.0003755321 | 323.15 | 0.8999 | 0.1001 | Yes |
| 5.23 | 0.0004257369 | 323.15 | 0.8999 | 0.1001 | Yes |
| 4.69 | 0.0004860366 | 323.15 | 0.8999 | 0.1001 | Yes |
| 4.16 | 0.0005614443 | 323.15 | 0.8999 | 0.1001 | Yes |
| 3.63 | 0.0006579570 | 323.15 | 0.8999 | 0.1001 | Yes |
| 3.11 | 0.0007851361 | 323.15 | 0.8999 | 0.1001 | Yes |
| 2.59 | 0.0009638354 | 323.15 | 0.8999 | 0.1001 | Yes |
| 2.08 | 0.0012248123 | 323.15 | 0.8999 | 0.1001 | Yes |
| 1.58 | 0.0016381235 | 323.15 | 0.8999 | 0.1001 | Yes |
| 21.48 | 0.0000613360 | 323.15 | 0.9246 | 0.0754 | Yes |
| 19.92 | 0.0000639381 | 323.15 | 0.9246 | 0.0754 | Yes |
| 18.63 | 0.0000666944 | 323.15 | 0.9246 | 0.0754 | Yes |
| 18.43 | 0.0000671771 | 323.15 | 0.9246 | 0.0754 | Yes |
| 17.53 | 0.0000696872 | 323.15 | 0.9246 | 0.0754 | Yes |
| 16.74 | 0.0000723922 | 323.15 | 0.9246 | 0.0754 | Yes |
| 16.57 | 0.0000730264 | 323.15 | 0.9246 | 0.0754 | Yes |
| 15.73 | 0.0000767161 | 323.15 | 0.9246 | 0.0754 | Yes |

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|--------------------------------------|---------------|-------------------|------------------|--------------------|
| 15.00 | 0.0000807666 | 323.15 | 0.9246 | 0.0754 | Yes |
| 14.45 | 0.0000843180 | 323.15 | 0.9246 | 0.0754 | Yes |
| 13.96 | 0.0000883488 | 323.15 | 0.9246 | 0.0754 | Yes |
| 13.53 | 0.0000925321 | 323.15 | 0.9246 | 0.0754 | Yes |
| 13.09 | 0.0000970389 | 323.15 | 0.9246 | 0.0754 | Yes |
| 12.73 | 0.0001019053 | 323.15 | 0.9246 | 0.0754 | Yes |
| 12.48 | 0.0001054030 | 323.15 | 0.9246 | 0.0754 | Yes |
| 12.31 | 0.0001073421 | 323.15 | 0.9246 | 0.0754 | Yes |
| 11.70 | 0.0001177390 | 323.15 | 0.9246 | 0.0754 | Yes |
| 11.06 | 0.0001308253 | 323.15 | 0.9246 | 0.0754 | Yes |
| 10.44 | 0.0001457141 | 323.15 | 0.9246 | 0.0754 | Yes |
| 9.87 | 0.0001613098 | 323.15 | 0.9246 | 0.0754 | Yes |
| 9.31 | 0.0001785905 | 323.15 | 0.9246 | 0.0754 | Yes |
| 8.75 | 0.0001984628 | 323.15 | 0.9246 | 0.0754 | Yes |
| 8.24 | 0.0002193537 | 323.15 | 0.9246 | 0.0754 | Yes |
| 7.73 | 0.0002428279 | 323.15 | 0.9246 | 0.0754 | Yes |
| 7.24 | 0.0002685316 | 323.15 | 0.9246 | 0.0754 | Yes |
| 6.72 | 0.0002990018 | 323.15 | 0.9246 | 0.0754 | Yes |
| 6.24 | 0.0003323324 | 323.15 | 0.9246 | 0.0754 | Yes |
| 5.69 | 0.0003760926 | 323.15 | 0.9246 | 0.0754 | Yes |
| 5.15 | 0.0004272349 | 323.15 | 0.9246 | 0.0754 | Yes |
| 4.62 | 0.0004891455 | 323.15 | 0.9246 | 0.0754 | Yes |
| 4.09 | 0.0005672730 | 323.15 | 0.9246 | 0.0754 | Yes |
| 3.57 | 0.0006652061 | 323.15 | 0.9246 | 0.0754 | Yes |
| 3.06 | 0.0007930806 | 323.15 | 0.9246 | 0.0754 | Yes |
| 2.54 | 0.0009747888 | 323.15 | 0.9246 | 0.0754 | Yes |
| 2.03 | 0.0012452333 | 323.15 | 0.9246 | 0.0754 | Yes |
| 1.53 | 0.0016877542 | 323.15 | 0.9246 | 0.0754 | Yes |
| 22.63 | 0.0000552842 | 323.15 | 0.9799 | 0.0201 | Yes |
| 20.78 | 0.0000569622 | 323.15 | 0.9799 | 0.0201 | Yes |
| 19.41 | 0.0000584508 | 323.15 | 0.9799 | 0.0201 | Yes |
| 18.02 | 0.0000602792 | 323.15 | 0.9799 | 0.0201 | Yes |
| 16.78 | 0.0000623965 | 323.15 | 0.9799 | 0.0201 | Yes |
| 16.68 | 0.0000626047 | 323.15 | 0.9799 | 0.0201 | Yes |
| 15.63 | 0.0000649698 | 323.15 | 0.9799 | 0.0201 | Yes |
| 14.69 | 0.0000677644 | 323.15 | 0.9799 | 0.0201 | Yes |
| 13.85 | 0.0000711253 | 323.15 | 0.9799 | 0.0201 | Yes |
| 13.10 | 0.0000753069 | 323.15 | 0.9799 | 0.0201 | Yes |
| 12.38 | 0.0000809563 | 323.15 | 0.9799 | 0.0201 | Yes |
| 12.43 | 0.0000805485 | 323.15 | 0.9799 | 0.0201 | Yes |
| 11.94 | 0.0000858511 | 323.15 | 0.9799 | 0.0201 | Yes |
| 11.45 | 0.0000931304 | 323.15 | 0.9799 | 0.0201 | Yes |
| 11.04 | 0.0001009729 | 323.15 | 0.9799 | 0.0201 | Yes |
| 10.65 | 0.0001102296 | 323.15 | 0.9799 | 0.0201 | Yes |
| 10.19 | 0.0001238620 | 323.15 | 0.9799 | 0.0201 | Yes |
| 9.85 | 0.0001351046 | 323.15 | 0.9799 | 0.0201 | Yes |
| 9.53 | 0.0001466234 | 323.15 | 0.9799 | 0.0201 | Yes |
| 9.19 | 0.0001599923 | 323.15 | 0.9799 | 0.0201 | Yes |
| 8.85 | 0.0001737059 | 323.15 | 0.9799 | 0.0201 | Yes |
| 8.54 | 0.0001866231 | 323.15 | 0.9799 | 0.0201 | Yes |
| 8.24 | 0.0001999348 | 323.15 | 0.9799 | 0.0201 | Yes |
| 7.95 | 0.0002132704 | 323.15 | 0.9799 | 0.0201 | Yes |
| 7.66 | 0.0002273087 | 323.15 | 0.9799 | 0.0201 | Yes |
| 7.25 | 0.0002492259 | 323.15 | 0.9799 | 0.0201 | Yes |
| 6.70 | 0.0002826845 | 323.15 | 0.9799 | 0.0201 | Yes |
| 6.23 | 0.0003148499 | 323.15 | 0.9799 | 0.0201 | Yes |
| 5.75 | 0.0003529511 | 323.15 | 0.9799 | 0.0201 | Yes |
| 5.23 | 0.0004019173 | 323.15 | 0.9799 | 0.0201 | Yes |
| 4.74 | 0.0004577510 | 323.15 | 0.9799 | 0.0201 | Yes |
| 4.22 | 0.0005296432 | 323.15 | 0.9799 | 0.0201 | Yes |
| 3.70 | 0.0006202000 | 323.15 | 0.9799 | 0.0201 | Yes |
| 3.19 | 0.0007378790 | 323.15 | 0.9799 | 0.0201 | Yes |
| 2.68 | 0.0009011674 | 323.15 | 0.9799 | 0.0201 | Yes |
| 2.20 | 0.0011241125 | 323.15 | 0.9799 | 0.0201 | Yes |
| 21.04 | 0.0000712731 | 333.15 | 0.9004 | 0.0996 | Yes |
| 19.98 | 0.0000742079 | 333.15 | 0.9004 | 0.0996 | Yes |
| 19.05 | 0.0000773047 | 333.15 | 0.9004 | 0.0996 | Yes |
| 18.16 | 0.0000807694 | 333.15 | 0.9004 | 0.0996 | Yes |
| 17.41 | 0.0000843801 | 333.15 | 0.9004 | 0.0996 | Yes |
| 16.74 | 0.0000880747 | 333.15 | 0.9004 | 0.0996 | Yes |
| 16.66 | 0.0000884267 | 333.15 | 0.9004 | 0.0996 | Yes |
| 16.06 | 0.0000923641 | 333.15 | 0.9004 | 0.0996 | Yes |
| 15.50 | 0.0000964344 | 333.15 | 0.9004 | 0.0996 | Yes |
| 14.97 | 0.0001008289 | 333.15 | 0.9004 | 0.0996 | Yes |
| 14.51 | 0.0001052243 | 333.15 | 0.9004 | 0.0996 | Yes |
| 14.10 | 0.0001095363 | 333.15 | 0.9004 | 0.0996 | Yes |
| 13.72 | 0.0001139554 | 333.15 | 0.9004 | 0.0996 | Yes |
| 13.44 | 0.0001175543 | 333.15 | 0.9004 | 0.0996 | Yes |
| 13.15 | 0.0001213510 | 333.15 | 0.9004 | 0.0996 | Yes |
| 12.51 | 0.0001311406 | 333.15 | 0.9004 | 0.0996 | Yes |
| 11.85 | 0.0001425462 | 333.15 | 0.9004 | 0.0996 | Yes |
| 11.25 | 0.0001541905 | 333.15 | 0.9004 | 0.0996 | Yes |
| 10.73 | 0.0001663634 | 333.15 | 0.9004 | 0.0996 | Yes |
| 10.16 | 0.0001805412 | 333.15 | 0.9004 | 0.0996 | Yes |
| 9.59 | 0.0001974586 | 333.15 | 0.9004 | 0.0996 | Yes |
| 9.04 | 0.0002156329 | 333.15 | 0.9004 | 0.0996 | Yes |
| 8.53 | 0.0002348314 | 333.15 | 0.9004 | 0.0996 | Yes |
| 8.00 | 0.0002574492 | 333.15 | 0.9004 | 0.0996 | Yes |
| 7.48 | 0.0002828650 | 333.15 | 0.9004 | 0.0996 | Yes |
| 6.99 | 0.0003106661 | 333.15 | 0.9004 | 0.0996 | Yes |
| 6.49 | 0.0003421598 | 333.15 | 0.9004 | 0.0996 | Yes |

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{H_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 5.96 | 0.0003818542 | 333.15 | 0.9004 | 0.0996 | Yes |
| 5.42 | 0.0004291745 | 333.15 | 0.9004 | 0.0996 | Yes |
| 4.89 | 0.0004862930 | 333.15 | 0.9004 | 0.0996 | Yes |
| 4.36 | 0.0005570265 | 333.15 | 0.9004 | 0.0996 | Yes |
| 3.84 | 0.0006465487 | 333.15 | 0.9004 | 0.0996 | Yes |
| 3.32 | 0.0007600648 | 333.15 | 0.9004 | 0.0996 | Yes |
| 2.84 | 0.0009051681 | 333.15 | 0.9004 | 0.0996 | Yes |
| 2.32 | 0.0011282549 | 333.15 | 0.9004 | 0.0996 | Yes |
| 1.82 | 0.0014642426 | 333.15 | 0.9004 | 0.0996 | Yes |
| 21.79 | 0.0000666400 | 333.15 | 0.9246 | 0.0754 | Yes |
| 20.59 | 0.0000692383 | 333.15 | 0.9246 | 0.0754 | Yes |
| 19.60 | 0.0000718320 | 333.15 | 0.9246 | 0.0754 | Yes |
| 18.63 | 0.0000749287 | 333.15 | 0.9246 | 0.0754 | Yes |
| 18.42 | 0.0000757065 | 333.15 | 0.9246 | 0.0754 | Yes |
| 17.36 | 0.0000801327 | 333.15 | 0.9246 | 0.0754 | Yes |
| 16.45 | 0.0000849847 | 333.15 | 0.9246 | 0.0754 | Yes |
| 16.24 | 0.0000861862 | 333.15 | 0.9246 | 0.0754 | Yes |
| 15.42 | 0.0000919074 | 333.15 | 0.9246 | 0.0754 | Yes |
| 14.82 | 0.0000969007 | 333.15 | 0.9246 | 0.0754 | Yes |
| 14.65 | 0.0000985372 | 333.15 | 0.9246 | 0.0754 | Yes |
| 14.11 | 0.0001040868 | 333.15 | 0.9246 | 0.0754 | Yes |
| 13.61 | 0.0001102095 | 333.15 | 0.9246 | 0.0754 | Yes |
| 13.15 | 0.0001163968 | 333.15 | 0.9246 | 0.0754 | Yes |
| 12.73 | 0.0001229860 | 333.15 | 0.9246 | 0.0754 | Yes |
| 12.35 | 0.0001295390 | 333.15 | 0.9246 | 0.0754 | Yes |
| 12.04 | 0.0001336507 | 333.15 | 0.9246 | 0.0754 | Yes |
| 11.89 | 0.0001363273 | 333.15 | 0.9246 | 0.0754 | Yes |
| 11.29 | 0.0001484684 | 333.15 | 0.9246 | 0.0754 | Yes |
| 10.70 | 0.0001620780 | 333.15 | 0.9246 | 0.0754 | Yes |
| 10.12 | 0.0001768123 | 333.15 | 0.9246 | 0.0754 | Yes |
| 9.55 | 0.0001932970 | 333.15 | 0.9246 | 0.0754 | Yes |
| 8.98 | 0.0002122851 | 333.15 | 0.9246 | 0.0754 | Yes |
| 8.42 | 0.0002331259 | 333.15 | 0.9246 | 0.0754 | Yes |
| 7.89 | 0.0002560731 | 333.15 | 0.9246 | 0.0754 | Yes |
| 7.37 | 0.0002816804 | 333.15 | 0.9246 | 0.0754 | Yes |
| 6.87 | 0.0003105981 | 333.15 | 0.9246 | 0.0754 | Yes |
| 6.38 | 0.0003420741 | 333.15 | 0.9246 | 0.0754 | Yes |
| 5.96 | 0.0003750565 | 333.15 | 0.9246 | 0.0754 | Yes |
| 5.43 | 0.0004223749 | 333.15 | 0.9246 | 0.0754 | Yes |
| 4.89 | 0.0004805136 | 333.15 | 0.9246 | 0.0754 | Yes |
| 4.36 | 0.0005519412 | 333.15 | 0.9246 | 0.0754 | Yes |
| 3.84 | 0.0006401826 | 333.15 | 0.9246 | 0.0754 | Yes |
| 3.33 | 0.0007535729 | 333.15 | 0.9246 | 0.0754 | Yes |
| 2.81 | 0.0009096582 | 333.15 | 0.9246 | 0.0754 | Yes |
| 2.30 | 0.0011345459 | 333.15 | 0.9246 | 0.0754 | Yes |
| 1.80 | 0.0014798425 | 333.15 | 0.9246 | 0.0754 | Yes |
| 20.76 | 0.0000619402 | 333.15 | 0.9802 | 0.0198 | Yes |
| 18.97 | 0.0000649790 | 333.15 | 0.9802 | 0.0198 | Yes |
| 17.44 | 0.0000685700 | 333.15 | 0.9802 | 0.0198 | Yes |
| 16.14 | 0.0000729490 | 333.15 | 0.9802 | 0.0198 | Yes |
| 16.12 | 0.0000730230 | 333.15 | 0.9802 | 0.0198 | Yes |
| 15.01 | 0.0000784208 | 333.15 | 0.9802 | 0.0198 | Yes |
| 14.05 | 0.0000850976 | 333.15 | 0.9802 | 0.0198 | Yes |
| 13.15 | 0.0000940913 | 333.15 | 0.9802 | 0.0198 | Yes |
| 12.40 | 0.0001046245 | 333.15 | 0.9802 | 0.0198 | Yes |
| 11.72 | 0.0001173011 | 333.15 | 0.9802 | 0.0198 | Yes |
| 10.87 | 0.0001369008 | 333.15 | 0.9802 | 0.0198 | Yes |
| 10.26 | 0.0001541539 | 333.15 | 0.9802 | 0.0198 | Yes |
| 9.59 | 0.0001750954 | 333.15 | 0.9802 | 0.0198 | Yes |
| 9.05 | 0.0001938865 | 333.15 | 0.9802 | 0.0198 | Yes |
| 8.95 | 0.0001976134 | 333.15 | 0.9802 | 0.0198 | Yes |
| 8.36 | 0.0002215419 | 333.15 | 0.9802 | 0.0198 | Yes |
| 7.69 | 0.0002519167 | 333.15 | 0.9802 | 0.0198 | Yes |
| 7.37 | 0.0002686902 | 333.15 | 0.9802 | 0.0198 | Yes |
| 7.17 | 0.0002800163 | 333.15 | 0.9802 | 0.0198 | Yes |
| 6.70 | 0.0003084180 | 333.15 | 0.9802 | 0.0198 | Yes |
| 6.19 | 0.0003437780 | 333.15 | 0.9802 | 0.0198 | Yes |
| 5.71 | 0.0003824492 | 333.15 | 0.9802 | 0.0198 | Yes |
| 5.26 | 0.0004262440 | 333.15 | 0.9802 | 0.0198 | Yes |
| 4.73 | 0.0004867928 | 333.15 | 0.9802 | 0.0198 | Yes |
| 4.21 | 0.0005614892 | 333.15 | 0.9802 | 0.0198 | Yes |
| 3.69 | 0.0006552127 | 333.15 | 0.9802 | 0.0198 | Yes |
| 3.18 | 0.0007793956 | 333.15 | 0.9802 | 0.0198 | Yes |
| 2.66 | 0.0009510687 | 333.15 | 0.9802 | 0.0198 | Yes |
| 2.16 | 0.0011994033 | 333.15 | 0.9802 | 0.0198 | Yes |
| 1.66 | 0.0015933033 | 333.15 | 0.9802 | 0.0198 | Yes |

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

7.1.5 Carbon Dioxide–Oxygen VLE Data

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | y_{CO_2} | y_{O_2} | Usable Data Point? |
|-------------|---|---|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 12.4163655 | — | — | 259.99 | — | — | 0.5 | 0.5 | No |
| 12.4163655 | — | — | 259.83 | — | — | 0.5 | 0.5 | No |
| 12.4163655 | — | — | 259.19 | — | — | 0.5 | 0.5 | No |
| 10.501323 | — | — | 258.53 | — | — | 0.5 | 0.5 | No |
| 13.326264 | — | — | 253.71 | — | — | 0.5 | 0.5 | No |
| 13.39415175 | — | — | 253.68 | — | — | 0.5 | 0.5 | No |
| 15.32945925 | — | — | 248.04 | — | — | 0.5 | 0.5 | No |
| 15.60405 | — | — | 244.77 | — | — | 0.5 | 0.5 | No |
| 13.9321875 | — | — | 244.11 | — | — | 0.5 | 0.5 | No |
| 14.20677825 | — | — | 243.47 | — | — | 0.5 | 0.5 | No |
| 13.9321875 | — | — | 243.47 | — | — | 0.5 | 0.5 | No |
| 13.9321875 | — | — | 242.95 | — | — | 0.5 | 0.5 | No |
| 14.0699895 | — | — | 242.95 | — | — | 0.5 | 0.5 | No |
| 14.0699895 | — | — | 242.83 | — | — | 0.5 | 0.5 | No |
| 14.1388905 | — | — | 240.11 | — | — | 0.5 | 0.5 | No |
| 14.20677825 | — | — | 239.71 | — | — | 0.5 | 0.5 | No |
| 14.20677825 | — | — | 239.77 | — | — | 0.5 | 0.5 | No |
| 3.61020975 | — | — | 239.65 | — | — | 0.5 | 0.5 | No |
| 3.61020975 | — | — | 239.55 | — | — | 0.5 | 0.5 | No |
| 14.2523745 | — | — | 237.93 | — | — | 0.5 | 0.5 | No |
| 14.27770575 | — | — | 237.44 | — | — | 0.5 | 0.5 | No |
| 14.26757325 | — | — | 237.28 | — | — | 0.5 | 0.5 | No |
| 14.331408 | — | — | 235.06 | — | — | 0.5 | 0.5 | No |
| 14.6211975 | — | — | 235.52 | — | — | 0.5 | 0.5 | No |
| 14.27770575 | — | — | 235.57 | — | — | 0.5 | 0.5 | No |
| 10.9370205 | — | — | 252.92 | — | — | 0.4 | 0.6 | No |
| 10.9370205 | — | — | 252.89 | — | — | 0.4 | 0.6 | No |
| 11.0059215 | — | — | 252.49 | — | — | 0.4 | 0.6 | No |
| 11.0059215 | — | — | 252.26 | — | — | 0.4 | 0.6 | No |
| 11.0059215 | — | — | 252.03 | — | — | 0.4 | 0.6 | No |
| 11.0059215 | — | — | 251.85 | — | — | 0.4 | 0.6 | No |
| 11.0059215 | — | — | 252.09 | — | — | 0.4 | 0.6 | No |
| 9.074667 | — | — | 252.59 | — | — | 0.4 | 0.6 | No |
| 9.08378625 | — | — | 252.75 | — | — | 0.4 | 0.6 | No |
| 11.8813695 | — | — | 251.83 | — | — | 0.4 | 0.6 | No |
| 11.9502705 | — | — | 251.86 | — | — | 0.4 | 0.6 | No |
| 12.01410525 | — | — | 251.93 | — | — | 0.4 | 0.6 | No |
| 12.14988075 | — | — | 251.9 | — | — | 0.4 | 0.6 | No |
| 9.074667 | — | — | 251.41 | — | — | 0.4 | 0.6 | No |
| 12.01410525 | — | — | 251.48 | — | — | 0.4 | 0.6 | No |
| 11.952297 | — | — | 251.31 | — | — | 0.4 | 0.6 | No |
| 11.91278025 | — | — | 251.48 | — | — | 0.4 | 0.6 | No |
| 12.14988075 | — | — | 250.66 | — | — | 0.4 | 0.6 | No |
| 12.14988075 | — | — | 250.89 | — | — | 0.4 | 0.6 | No |
| 13.05167325 | — | — | 248.18 | — | — | 0.4 | 0.6 | No |
| 13.08207075 | — | — | 248.18 | — | — | 0.4 | 0.6 | No |
| 13.6444245 | — | — | 242.16 | — | — | 0.4 | 0.6 | No |
| 13.909896 | — | — | 242.16 | — | — | 0.4 | 0.6 | No |
| 13.909896 | — | — | 242.23 | — | — | 0.4 | 0.6 | No |
| 13.8713925 | — | — | 242.2 | — | — | 0.4 | 0.6 | No |
| 13.88659125 | — | — | 242.03 | — | — | 0.4 | 0.6 | No |
| 14.29189125 | — | — | 235.87 | — | — | 0.4 | 0.6 | No |
| 14.32228875 | — | — | 235.9 | — | — | 0.4 | 0.6 | No |
| 14.30709 | — | — | 235.9 | — | — | 0.4 | 0.6 | No |
| 14.30709 | — | — | 235.83 | — | — | 0.4 | 0.6 | No |
| 3.611223 | — | — | 233.97 | — | — | 0.4 | 0.6 | No |
| 3.611223 | — | — | 234.4 | — | — | 0.4 | 0.6 | No |
| 9.743412 | — | — | 240.18 | — | — | 0.3 | 0.7 | No |
| 9.743412 | — | — | 240.01 | — | — | 0.3 | 0.7 | No |
| 11.60272575 | — | — | 239.51 | — | — | 0.3 | 0.7 | No |
| 11.67162675 | — | — | 239.51 | — | — | 0.3 | 0.7 | No |
| 11.63312325 | — | — | 239.35 | — | — | 0.3 | 0.7 | No |
| 11.63312325 | — | — | 239.51 | — | — | 0.3 | 0.7 | No |
| 11.648322 | — | — | 239.51 | — | — | 0.3 | 0.7 | No |
| 11.66352075 | — | — | 239.51 | — | — | 0.3 | 0.7 | No |
| 10.77591375 | — | — | 241.01 | — | — | 0.3 | 0.7 | No |
| 10.77591375 | — | — | 240.84 | — | — | 0.3 | 0.7 | No |
| 11.05354425 | — | — | 240.61 | — | — | 0.3 | 0.7 | No |
| 11.05354425 | — | — | 240.71 | — | — | 0.3 | 0.7 | No |
| 10.432422 | — | — | 240.84 | — | — | 0.3 | 0.7 | No |
| 10.432422 | — | — | 240.94 | — | — | 0.3 | 0.7 | No |
| 9.123303 | — | — | 240.84 | — | — | 0.3 | 0.7 | No |
| 9.123303 | — | — | 241.18 | — | — | 0.3 | 0.7 | No |
| 12.91387125 | — | — | 235.22 | — | — | 0.3 | 0.7 | No |
| 13.05167325 | — | — | 235.22 | — | — | 0.3 | 0.7 | No |
| 13.7416965 | — | — | 233.08 | — | — | 0.3 | 0.7 | No |
| 13.8105975 | — | — | 233.74 | — | — | 0.3 | 0.7 | No |
| 5.333748 | — | — | 232.23 | — | — | 0.3 | 0.7 | No |
| 5.333748 | — | — | 232.07 | — | — | 0.3 | 0.7 | No |

Data summarised from TABLE I, II, III, IV, and V of Booth30 [76]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | y_{CO_2} | y_{O_2} | Usable Data Point? |
|-------------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 10.5033495 | — | — | 228.29 | — | — | 0.2 | 0.8 | No |
| 10.5033495 | — | — | 228.22 | — | — | 0.2 | 0.8 | No |
| 11.1923595 | — | — | 223.25 | — | — | 0.2 | 0.8 | No |
| 11.2612605 | — | — | 223.31 | — | — | 0.2 | 0.8 | No |
| 11.1923595 | — | — | 223.21 | — | — | 0.2 | 0.8 | No |
| 11.2612605 | — | — | 223.25 | — | — | 0.2 | 0.8 | No |
| 10.19228175 | — | — | 224.39 | — | — | 0.2 | 0.8 | No |
| 10.19228175 | — | — | 224.92 | — | — | 0.2 | 0.8 | No |
| 10.19228175 | — | — | 224.42 | — | — | 0.2 | 0.8 | No |
| 10.19228175 | — | — | 223.28 | — | — | 0.2 | 0.8 | No |
| 10.8073245 | — | — | 223.38 | — | — | 0.2 | 0.8 | No |
| 5.333748 | — | — | 219.58 | — | — | 0.2 | 0.8 | No |
| 5.333748 | — | — | 219.65 | — | — | 0.2 | 0.8 | No |
| 11.7840975 | — | — | 221.09 | — | — | 0.2 | 0.8 | No |
| 11.7840975 | — | — | 220.99 | — | — | 0.2 | 0.8 | No |
| 12.8338245 | — | — | 215.27 | — | — | 0.2 | 0.8 | No |
| 12.8946195 | — | — | 215.27 | — | — | 0.2 | 0.8 | No |
| 3.509898 | — | — | 214.76 | — | — | 0.2 | 0.8 | No |
| 7.056273 | — | — | 213.25 | — | — | 0.2 | 0.8 | No |
| 13.14083925 | — | — | 212.89 | — | — | 0.2 | 0.8 | No |
| 13.103349 | — | — | 212.89 | — | — | 0.2 | 0.8 | No |
| 13.11854775 | — | — | 212.82 | — | — | 0.2 | 0.8 | No |
| 13.20974025 | — | — | 212.17 | — | — | 0.2 | 0.8 | No |
| 13.14083925 | — | — | 211.88 | — | — | 0.2 | 0.8 | No |
| 13.20974025 | — | — | 210.58 | — | — | 0.2 | 0.8 | No |
| 13.20974025 | — | — | 210.41 | — | — | 0.2 | 0.8 | No |
| 14.26554675 | — | — | 210.58 | — | — | 0.2 | 0.8 | No |
| 13.20974025 | — | — | 212.76 | — | — | 0.2 | 0.8 | No |
| 13.27053525 | — | — | 212.76 | — | — | 0.2 | 0.8 | No |
| 13.20974025 | — | — | 211.13 | — | — | 0.2 | 0.8 | No |
| 13.19960775 | — | — | 211.06 | — | — | 0.2 | 0.8 | No |
| 13.19960775 | — | — | 210.84 | — | — | 0.2 | 0.8 | No |
| 7.056273 | — | — | 212.88 | — | — | 0.2 | 0.8 | No |
| 7.056273 | — | — | 213.25 | — | — | 0.2 | 0.8 | No |
| 7.056273 | — | — | 213.08 | — | — | 0.2 | 0.8 | No |
| 7.056273 | — | — | 209.04 | — | — | 0.1 | 0.9 | No |
| 7.056273 | — | — | 208.07 | — | — | 0.1 | 0.9 | No |
| 8.778798 | — | — | 207.91 | — | — | 0.1 | 0.9 | No |
| 8.778798 | — | — | 207.84 | — | — | 0.1 | 0.9 | No |
| 8.778798 | — | — | 207.98 | — | — | 0.1 | 0.9 | No |
| 10.501323 | — | — | 205.92 | — | — | 0.1 | 0.9 | No |
| 10.501323 | — | — | 205.89 | — | — | 0.1 | 0.9 | No |
| 10.501323 | — | — | 205.79 | — | — | 0.1 | 0.9 | No |
| 13.946373 | — | — | 202.18 | — | — | 0.1 | 0.9 | No |
| 13.946373 | — | — | 202.15 | — | — | 0.1 | 0.9 | No |

Continued: Data summarised from TABLE I, II, III, IV, and V of Booth30 [76]

| P (MPa) | v_{Bub} ($\text{m}^3\text{mol}^{-1}$) | v_{Dew} ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | y_{CO_2} | y_{O_2} | Usable Data Point? |
|-----------|--|--|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 0.93118 | — | — | 223.75 | 0.9960 | 0.0040 | 0.7778 | 0.2222 | Vol. Est. |
| 1.42666 | — | — | 223.75 | 0.9878 | 0.0122 | 0.5539 | 0.4461 | Vol. Est. |
| 2.59392 | — | — | 223.75 | 0.9694 | 0.0306 | 0.3547 | 0.6453 | Vol. Est. |
| 3.42479 | — | — | 223.75 | 0.9574 | 0.0426 | 0.2899 | 0.7101 | Vol. Est. |
| 5.04599 | — | — | 223.75 | 0.9244 | 0.0756 | 0.2229 | 0.7771 | Vol. Est. |
| 7.75136 | — | — | 223.75 | 0.8567 | 0.1433 | 0.1863 | 0.8137 | Vol. Est. |
| 8.71395 | — | — | 223.75 | 0.8192 | 0.1808 | — | — | No |
| 11.85503 | — | — | 223.75 | 0.6944 | 0.3056 | 0.2030 | 0.7970 | Vol. Est. |
| 12.72642 | — | — | 223.75 | 0.6587 | 0.3413 | 0.2192 | 0.7808 | Vol. Est. |
| 13.78020 | — | — | 223.75 | 0.6071 | 0.3929 | 0.2887 | 0.7113 | Vol. Est. |
| 14.23616 | — | — | 223.75 | 0.5538 | 0.4462 | 0.3760 | 0.6240 | Vol. Est. |

Data summarised from Table I of Fredenslund72 [123]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | $T(\text{K})$ | x_{CO_2} | x_{O_2} | y_{CO_2} | y_{O_2} | Usable Data Point? |
|-----------|---|---|---------------|-------------------|------------------|-------------------|------------------|--------------------|
| 1.01325 | — | — | 223.15 | 0.992 | 0.008 | 0.688 | 0.312 | Vol. Est. |
| 2.02650 | — | — | 223.15 | 0.975 | 0.025 | 0.383 | 0.617 | Vol. Est. |
| 3.03975 | — | — | 223.15 | 0.951 | 0.049 | 0.288 | 0.712 | Vol. Est. |
| 4.05300 | — | — | 223.15 | 0.929 | 0.071 | 0.239 | 0.761 | Vol. Est. |
| 5.06625 | — | — | 223.15 | 0.904 | 0.096 | 0.211 | 0.789 | Vol. Est. |
| 6.07950 | — | — | 223.15 | 0.883 | 0.117 | 0.191 | 0.809 | Vol. Est. |
| 7.09275 | — | — | 223.15 | 0.85 | 0.15 | 0.186 | 0.814 | Vol. Est. |
| 8.10600 | — | — | 223.15 | 0.811 | 0.189 | 0.182 | 0.818 | Vol. Est. |
| 9.11925 | — | — | 223.15 | 0.78 | 0.22 | 0.18 | 0.82 | Vol. Est. |
| 10.13250 | — | — | 223.15 | 0.733 | 0.267 | 0.181 | 0.819 | Vol. Est. |
| 11.14575 | — | — | 223.15 | 0.707 | 0.293 | 0.203 | 0.797 | Vol. Est. |
| 12.15900 | — | — | 223.15 | 0.666 | 0.334 | 0.22 | 0.78 | Vol. Est. |
| 13.17225 | — | — | 223.15 | 0.607 | 0.393 | 0.238 | 0.762 | Vol. Est. |
| 1.01325 | — | — | 233.15 | — | — | 0.882 | 0.118 | No |
| 2.02650 | — | — | 233.15 | 0.979 | 0.021 | 0.581 | 0.419 | Vol. Est. |
| 3.03975 | — | — | 233.15 | 0.959 | 0.041 | 0.411 | 0.589 | Vol. Est. |
| 4.05300 | — | — | 233.15 | 0.936 | 0.064 | 0.349 | 0.651 | Vol. Est. |
| 5.06625 | — | — | 233.15 | 0.913 | 0.087 | 0.305 | 0.695 | Vol. Est. |
| 6.07950 | — | — | 233.15 | 0.88 | 0.12 | 0.277 | 0.723 | Vol. Est. |
| 7.09275 | — | — | 233.15 | 0.859 | 0.141 | 0.259 | 0.741 | Vol. Est. |
| 8.10600 | — | — | 233.15 | 0.833 | 0.167 | 0.243 | 0.757 | Vol. Est. |
| 9.11925 | — | — | 233.15 | 0.795 | 0.205 | 0.234 | 0.766 | Vol. Est. |
| 10.13250 | — | — | 233.15 | 0.752 | 0.248 | 0.233 | 0.767 | Vol. Est. |
| 11.14575 | — | — | 233.15 | 0.726 | 0.274 | 0.24 | 0.76 | Vol. Est. |
| 12.15900 | — | — | 233.15 | 0.672 | 0.328 | 0.27 | 0.73 | Vol. Est. |
| 13.17225 | — | — | 233.15 | 0.62 | 0.38 | 0.298 | 0.702 | Vol. Est. |
| 2.02650 | — | — | 243.15 | 0.99 | 0.01 | 0.725 | 0.275 | Vol. Est. |
| 3.03975 | — | — | 243.15 | 0.969 | 0.031 | 0.537 | 0.463 | Vol. Est. |
| 4.05300 | — | — | 243.15 | 0.948 | 0.052 | 0.449 | 0.551 | Vol. Est. |
| 5.06625 | — | — | 243.15 | 0.92 | 0.08 | 0.391 | 0.609 | Vol. Est. |
| 6.07950 | — | — | 243.15 | 0.896 | 0.104 | 0.356 | 0.644 | Vol. Est. |
| 7.09275 | — | — | 243.15 | 0.86 | 0.14 | 0.329 | 0.671 | Vol. Est. |
| 8.10600 | — | — | 243.15 | 0.838 | 0.162 | 0.307 | 0.693 | Vol. Est. |
| 9.11925 | — | — | 243.15 | 0.809 | 0.191 | 0.311 | 0.689 | Vol. Est. |
| 10.13250 | — | — | 243.15 | 0.764 | 0.236 | 0.306 | 0.694 | Vol. Est. |
| 11.14575 | — | — | 243.15 | 0.734 | 0.266 | 0.318 | 0.682 | Vol. Est. |
| 12.15900 | — | — | 243.15 | 0.694 | 0.306 | 0.329 | 0.671 | Vol. Est. |
| 2.02650 | — | — | 253.15 | 0.994 | 0.006 | 0.939 | 0.061 | Vol. Est. |
| 3.03975 | — | — | 253.15 | 0.97 | 0.03 | 0.698 | 0.302 | Vol. Est. |
| 4.05300 | — | — | 253.15 | 0.958 | 0.042 | 0.6 | 0.4 | Vol. Est. |
| 5.06625 | — | — | 253.15 | 0.938 | 0.062 | 0.5 | 0.5 | Vol. Est. |
| 6.07950 | — | — | 253.15 | 0.908 | 0.092 | 0.46 | 0.54 | Vol. Est. |
| 7.09275 | — | — | 253.15 | 0.875 | 0.125 | 0.44 | 0.56 | Vol. Est. |
| 8.10600 | — | — | 253.15 | 0.859 | 0.141 | 0.426 | 0.574 | Vol. Est. |
| 9.11925 | — | — | 253.15 | 0.83 | 0.17 | 0.399 | 0.601 | Vol. Est. |
| 10.13250 | — | — | 253.15 | 0.78 | 0.22 | 0.401 | 0.599 | Vol. Est. |
| 11.14575 | — | — | 253.15 | 0.745 | 0.255 | 0.399 | 0.601 | Vol. Est. |
| 12.15900 | — | — | 253.15 | 0.7 | 0.3 | 0.43 | 0.57 | Vol. Est. |
| 3.03975 | — | — | 263.15 | 0.991 | 0.009 | 0.904 | 0.096 | Vol. Est. |
| 4.05300 | — | — | 263.15 | 0.965 | 0.035 | 0.737 | 0.263 | Vol. Est. |
| 5.06625 | — | — | 263.15 | 0.944 | 0.056 | 0.654 | 0.346 | Vol. Est. |
| 6.07950 | — | — | 263.15 | 0.921 | 0.079 | 0.583 | 0.417 | Vol. Est. |
| 7.09275 | — | — | 263.15 | 0.89 | 0.11 | 0.537 | 0.463 | Vol. Est. |
| 8.10600 | — | — | 263.15 | 0.866 | 0.134 | 0.507 | 0.493 | Vol. Est. |
| 9.11925 | — | — | 263.15 | 0.838 | 0.162 | 0.505 | 0.495 | Vol. Est. |
| 10.13250 | — | — | 263.15 | 0.805 | 0.195 | 0.5 | 0.5 | Vol. Est. |
| 11.14575 | — | — | 263.15 | 0.757 | 0.243 | 0.502 | 0.498 | Vol. Est. |
| 12.15900 | — | — | 263.15 | 0.701 | 0.299 | 0.554 | 0.446 | Vol. Est. |
| 4.05300 | — | — | 273.15 | 0.99 | 0.01 | 0.901 | 0.099 | Vol. Est. |
| 5.06625 | — | — | 273.15 | 0.958 | 0.042 | 0.786 | 0.214 | Vol. Est. |
| 6.07950 | — | — | 273.15 | 0.938 | 0.062 | 0.702 | 0.298 | Vol. Est. |
| 7.09275 | — | — | 273.15 | 0.91 | 0.09 | 0.664 | 0.336 | Vol. Est. |
| 8.10600 | — | — | 273.15 | 0.874 | 0.126 | 0.628 | 0.372 | Vol. Est. |
| 9.11925 | — | — | 273.15 | 0.853 | 0.147 | 0.602 | 0.398 | Vol. Est. |
| 10.13250 | — | — | 273.15 | 0.815 | 0.185 | 0.599 | 0.401 | Vol. Est. |
| 11.14575 | — | — | 273.15 | 0.753 | 0.247 | 0.638 | 0.362 | Vol. Est. |
| 5.06625 | — | — | 283.15 | 0.972 | 0.028 | 0.885 | 0.115 | Vol. Est. |
| 6.07950 | — | — | 283.15 | 0.96 | 0.04 | 0.839 | 0.161 | Vol. Est. |
| 7.09275 | — | — | 283.15 | 0.929 | 0.071 | 0.782 | 0.218 | Vol. Est. |
| 8.10600 | — | — | 283.15 | 0.913 | 0.087 | 0.737 | 0.263 | Vol. Est. |
| 9.11925 | — | — | 283.15 | 0.885 | 0.115 | 0.706 | 0.294 | Vol. Est. |
| 10.13250 | — | — | 283.15 | 0.813 | 0.187 | 0.737 | 0.263 | Vol. Est. |

Data summarised from Table I of Fredenslund70 [112]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | y_{CO_2} | y_{O_2} | |
|-----------|---|---|---------|-------------------|------------------|-------------------|------------------|-----|
| 3.48530 | 0.00004735 | 0.0004505 | 273.15 | 1.0000 | 0.0000 | 1.0000 | 0.0000 | Yes |
| 3.79212 | 0.00004750 | 0.0004250 | 273.15 | 0.9934 | 0.0066 | 0.9520 | 0.0480 | Yes |
| 4.13685 | 0.00004700 | 0.0003980 | 273.15 | 0.9859 | 0.0141 | 0.9010 | 0.0990 | Yes |
| 4.48159 | 0.00004790 | 0.0003690 | 273.15 | 0.9782 | 0.0218 | 0.8550 | 0.1450 | Yes |
| 4.82633 | 0.00004810 | 0.0003410 | 273.15 | 0.9705 | 0.0295 | 0.8150 | 0.1850 | Yes |
| 5.17107 | 0.00004834 | 0.0003180 | 273.15 | 0.9625 | 0.0375 | 0.7782 | 0.2218 | Yes |
| 5.51581 | 0.00004858 | 0.0002960 | 273.15 | 0.9545 | 0.0455 | 0.7480 | 0.2520 | Yes |
| 5.86054 | 0.00004883 | 0.0002760 | 273.15 | 0.9461 | 0.0539 | 0.7225 | 0.2775 | Yes |
| 6.20528 | 0.00004911 | 0.0002570 | 273.15 | 0.9378 | 0.0622 | 0.7008 | 0.2992 | Yes |
| 6.55002 | 0.00004941 | 0.0002410 | 273.15 | 0.9290 | 0.0710 | 0.6820 | 0.3180 | Yes |
| 6.89476 | 0.00004974 | 0.0002260 | 273.15 | 0.9199 | 0.0801 | 0.6658 | 0.3342 | Yes |
| 7.23950 | 0.00005007 | 0.0002120 | 273.15 | 0.9101 | 0.0899 | 0.6512 | 0.3488 | Yes |
| 7.58423 | 0.00005045 | 0.0002010 | 273.15 | 0.9003 | 0.0997 | 0.6383 | 0.3617 | Yes |
| 7.92897 | 0.00005086 | 0.0001900 | 273.15 | 0.8901 | 0.1099 | 0.6268 | 0.3732 | Yes |
| 8.27371 | 0.00005131 | 0.0001800 | 273.15 | 0.8795 | 0.1205 | 0.6162 | 0.3838 | Yes |
| 8.61845 | 0.00005182 | 0.0001710 | 273.15 | 0.8680 | 0.1320 | 0.6070 | 0.3930 | Yes |
| 8.96318 | 0.00005239 | 0.0001620 | 273.15 | 0.8560 | 0.1440 | 0.5991 | 0.4009 | Yes |
| 9.30792 | 0.00005300 | 0.0001530 | 273.15 | 0.8435 | 0.1565 | 0.5940 | 0.4060 | Yes |
| 9.65266 | 0.00005368 | 0.0001440 | 273.15 | 0.8300 | 0.1700 | 0.5915 | 0.4085 | Yes |
| 9.99740 | 0.00005445 | 0.0001350 | 273.15 | 0.8165 | 0.1835 | 0.5915 | 0.4085 | Yes |
| 10.34214 | 0.00005540 | 0.0001260 | 273.15 | 0.8020 | 0.1980 | 0.5935 | 0.4065 | Yes |
| 10.68687 | 0.00005650 | 0.0001170 | 273.15 | 0.7861 | 0.2139 | 0.5980 | 0.4020 | Yes |
| 11.03161 | 0.00005795 | 0.0001080 | 273.15 | 0.7685 | 0.2315 | 0.6080 | 0.3920 | Yes |
| 11.37635 | 0.00006040 | 0.0000998 | 273.15 | 0.7485 | 0.2515 | 0.6250 | 0.3750 | Yes |
| 11.54872 | 0.00006230 | 0.0000938 | 273.15 | 0.7340 | 0.2660 | 0.6405 | 0.3595 | Yes |
| 11.74177 | 0.00007600 | 0.0000760 | 273.15 | 0.6880 | 0.3120 | 0.6880 | 0.3120 | Yes |

Data summarised from Table IV of Muirbrook64 [54]

| P (MPa) | v_{Bub} ($\text{m}^3 \text{mol}^{-1}$) | v_{Dew} ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | y_{CO_2} | y_{O_2} | Usable Data Point? |
|-------------|---|---|---------|-------------------|------------------|-------------------|------------------|--------------------|
| 6.028838095 | — | — | 273.15 | 0.9199 | 0.0801 | 0.6980 | 0.3020 | Vol. Est. |
| 6.099765602 | — | — | 273.15 | 0.9370 | 0.0630 | 0.6980 | 0.3020 | Vol. Est. |
| 6.018705594 | — | — | 273.15 | 0.9397 | 0.0603 | 0.7020 | 0.2980 | Vol. Est. |
| 5.319563025 | — | — | 273.15 | 0.9568 | 0.0432 | 0.7460 | 0.2540 | Vol. Est. |
| 6.971160688 | — | — | 273.15 | 0.9157 | 0.0843 | 0.6470 | 0.3530 | Vol. Est. |
| 8.491035838 | — | — | 273.15 | 0.8707 | 0.1293 | 0.5930 | 0.4070 | Vol. Est. |
| 9.42322593 | — | — | 273.15 | 0.8400 | 0.1600 | 0.5795 | 0.4205 | Vol. Est. |
| 10.40607853 | — | — | 273.15 | 0.8015 | 0.1985 | 0.5780 | 0.4220 | Vol. Est. |
| 11.1052211 | — | — | 273.15 | 0.7630 | 0.2370 | 0.6010 | 0.3990 | Vol. Est. |
| 13.87139387 | — | — | 232.85 | 0.5980 | 0.4020 | 0.2370 | 0.7630 | Vol. Est. |
| 12.39204872 | — | — | 232.85 | 0.6690 | 0.3310 | — | — | No |
| 12.53390374 | — | — | 232.85 | 0.6600 | 0.3400 | 0.2800 | 0.7200 | Vol. Est. |
| 11.1457511 | — | — | 232.85 | 0.7240 | 0.2760 | 0.2470 | 0.7530 | Vol. Est. |
| 9.463755934 | — | — | 232.85 | 0.7830 | 0.2170 | 0.2320 | 0.7680 | Vol. Est. |
| 7.771628267 | — | — | 232.85 | 0.8355 | 0.1645 | 0.2300 | 0.7700 | Vol. Est. |
| 13.48635883 | — | — | 232.85 | 0.5970 | 0.4030 | 0.2930 | 0.7070 | Vol. Est. |
| 14.77318646 | — | — | 232.85 | 0.4690 | 0.5310 | — | — | No |
| 14.87451147 | — | — | 232.85 | — | — | 0.4560 | 0.5440 | No |
| 14.29695891 | — | — | 232.85 | 0.5030 | 0.4970 | 0.3830 | 0.6170 | Vol. Est. |
| 5.917380584 | — | — | 232.85 | 0.8870 | 0.1130 | 0.2260 | 0.7740 | Vol. Est. |
| 7.275135718 | — | — | 232.85 | — | — | 0.2300 | 0.7700 | No |
| 4.924395486 | — | — | 232.85 | — | — | 0.2510 | 0.7490 | No |
| 3.789555374 | — | — | 232.85 | — | — | 0.2840 | 0.7160 | No |
| 2.664847763 | — | — | 232.85 | — | — | 0.4470 | 0.5530 | No |
| 3.85035038 | — | — | 232.85 | — | — | 0.3290 | 0.6710 | No |
| 2.188620216 | — | — | 218.15 | 0.9670 | 0.0330 | 0.2960 | 0.7040 | Vol. Est. |
| 3.941542889 | — | — | 218.15 | 0.9280 | 0.0720 | 0.1880 | 0.8120 | Vol. Est. |
| 5.907248083 | — | — | 218.15 | 0.8810 | 0.1190 | 0.1530 | 0.8470 | Vol. Est. |
| 7.883085778 | — | — | 218.15 | 0.8260 | 0.1740 | 0.1470 | 0.8530 | Vol. Est. |
| 9.717068459 | — | — | 218.15 | 0.7660 | 0.2340 | 0.1490 | 0.8510 | Vol. Est. |
| 11.82462867 | — | — | 218.15 | 0.6880 | 0.3120 | 0.1780 | 0.8220 | Vol. Est. |
| 13.01013128 | — | — | 218.15 | 0.6180 | 0.3820 | 0.2110 | 0.7890 | Vol. Est. |
| 14.02338138 | — | — | 218.15 | 0.5320 | 0.4680 | 0.2640 | 0.7360 | Vol. Est. |

Data summarised from TABLE 1 of Zenner63 [103]

7.1.6 Carbon Dioxide–Oxygen Density Data

| P (MPa) | v ($\text{m}^3\text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | Usable Data Point? |
|-----------|-------------------------------------|---------|-------------------|------------------|--------------------|
| 1.003 | 0.002413887 | 303.22 | 0.9393 | 0.0607 | Yes |
| 2.004 | 0.001157555 | 303.22 | 0.9393 | 0.0607 | Yes |
| 3.000 | 0.000725096 | 303.22 | 0.9393 | 0.0607 | Yes |
| 4.000 | 0.000510389 | 303.22 | 0.9393 | 0.0607 | Yes |
| 5.002 | 0.000377868 | 303.22 | 0.9393 | 0.0607 | Yes |
| 6.003 | 0.000284668 | 303.22 | 0.9393 | 0.0607 | Yes |
| 7.000 | 0.000212568 | 303.22 | 0.9393 | 0.0607 | Yes |
| 8.001 | 0.000149399 | 303.22 | 0.9393 | 0.0607 | Yes |
| 9.002 | 9.38565E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 10.001 | 7.35358E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 11.002 | 6.63849E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 12.004 | 6.25647E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 13.000 | 5.99933E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 14.000 | 5.82109E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 15.002 | 5.68231E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 16.001 | 5.56647E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 17.001 | 5.46871E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 18.001 | 5.37799E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 19.006 | 5.30034E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 20.003 | 5.23691E-05 | 303.22 | 0.9393 | 0.0607 | Yes |
| 1.000 | 0.002577784 | 323.18 | 0.9393 | 0.0607 | Yes |
| 2.003 | 0.001243349 | 323.18 | 0.9393 | 0.0607 | Yes |
| 3.003 | 0.000797365 | 323.18 | 0.9393 | 0.0607 | Yes |
| 4.002 | 0.000572122 | 323.18 | 0.9393 | 0.0607 | Yes |
| 5.001 | 0.000435729 | 323.18 | 0.9393 | 0.0607 | Yes |
| 6.001 | 0.000343092 | 323.18 | 0.9393 | 0.0607 | Yes |
| 7.003 | 0.000275693 | 323.18 | 0.9393 | 0.0607 | Yes |
| 8.001 | 0.000223883 | 323.18 | 0.9393 | 0.0607 | Yes |
| 9.001 | 0.000182289 | 323.18 | 0.9393 | 0.0607 | Yes |
| 10.001 | 0.000148421 | 323.18 | 0.9393 | 0.0607 | Yes |
| 11.000 | 0.000121552 | 323.18 | 0.9393 | 0.0607 | Yes |
| 12.001 | 0.000101589 | 323.18 | 0.9393 | 0.0607 | Yes |
| 13.000 | 8.80984E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 14.000 | 7.96031E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 15.001 | 7.37514E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 16.001 | 6.97203E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 17.001 | 6.67886E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 18.000 | 6.4459E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 19.001 | 6.25936E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 20.003 | 6.10073E-05 | 323.18 | 0.9393 | 0.0607 | Yes |
| 1.020 | 0.002834381 | 343.15 | 0.9393 | 0.0607 | Yes |
| 2.006 | 0.0013649 | 343.15 | 0.9393 | 0.0607 | Yes |
| 3.001 | 0.000886542 | 343.15 | 0.9393 | 0.0607 | Yes |
| 4.010 | 0.000643871 | 343.15 | 0.9393 | 0.0607 | Yes |
| 5.002 | 0.000489051 | 343.15 | 0.9393 | 0.0607 | Yes |
| 6.001 | 0.000391082 | 343.15 | 0.9393 | 0.0607 | Yes |
| 7.001 | 0.000320933 | 343.15 | 0.9393 | 0.0607 | Yes |
| 8.003 | 0.000268726 | 343.15 | 0.9393 | 0.0607 | Yes |
| 9.001 | 0.000227939 | 343.15 | 0.9393 | 0.0607 | Yes |
| 10.003 | 0.000194951 | 343.15 | 0.9393 | 0.0607 | Yes |
| 11.000 | 0.000168225 | 343.15 | 0.9393 | 0.0607 | Yes |
| 12.001 | 0.000146601 | 343.15 | 0.9393 | 0.0607 | Yes |
| 13.001 | 0.000128816 | 343.15 | 0.9393 | 0.0607 | Yes |
| 14.002 | 0.000114536 | 343.15 | 0.9393 | 0.0607 | Yes |
| 15.003 | 0.000103397 | 343.15 | 0.9393 | 0.0607 | Yes |
| 16.001 | 9.45847E-05 | 343.15 | 0.9393 | 0.0607 | Yes |
| 17.001 | 8.76435E-05 | 343.15 | 0.9393 | 0.0607 | Yes |
| 18.002 | 8.236E-05 | 343.15 | 0.9393 | 0.0607 | Yes |
| 19.002 | 7.81584E-05 | 343.15 | 0.9393 | 0.0607 | Yes |
| 20.002 | 7.47358E-05 | 343.15 | 0.9393 | 0.0607 | Yes |
| 1.004 | 0.003147709 | 363.15 | 0.9393 | 0.0607 | Yes |
| 2.010 | 0.001457763 | 363.15 | 0.9393 | 0.0607 | Yes |
| 3.011 | 0.000960732 | 363.15 | 0.9393 | 0.0607 | Yes |
| 4.006 | 0.000690617 | 363.15 | 0.9393 | 0.0607 | Yes |
| 5.000 | 0.000531185 | 363.15 | 0.9393 | 0.0607 | Yes |
| 6.000 | 0.000429588 | 363.15 | 0.9393 | 0.0607 | Yes |
| 7.003 | 0.000358881 | 363.15 | 0.9393 | 0.0607 | Yes |
| 8.002 | 0.000304431 | 363.15 | 0.9393 | 0.0607 | Yes |
| 9.004 | 0.000262627 | 363.15 | 0.9393 | 0.0607 | Yes |
| 10.002 | 0.000229012 | 363.15 | 0.9393 | 0.0607 | Yes |
| 11.001 | 0.000201795 | 363.15 | 0.9393 | 0.0607 | Yes |
| 12.000 | 0.000179306 | 363.15 | 0.9393 | 0.0607 | Yes |
| 13.001 | 0.00016046 | 363.15 | 0.9393 | 0.0607 | Yes |
| 14.000 | 0.00014469 | 363.15 | 0.9393 | 0.0607 | Yes |
| 15.003 | 0.000131461 | 363.15 | 0.9393 | 0.0607 | Yes |
| 16.001 | 0.000120483 | 363.15 | 0.9393 | 0.0607 | Yes |
| 17.001 | 0.000111317 | 363.15 | 0.9393 | 0.0607 | Yes |
| 18.001 | 0.000103687 | 363.15 | 0.9393 | 0.0607 | Yes |
| 19.001 | 9.73328E-05 | 363.15 | 0.9393 | 0.0607 | Yes |
| 20.003 | 9.18585E-05 | 363.15 | 0.9393 | 0.0607 | Yes |

Data summarised from Table 6 and 7 of Mantovani12 [109]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 1.009 | 0.003376052 | 383.14 | 0.9393 | 0.0607 | Yes |
| 2.002 | 0.001594143 | 383.14 | 0.9393 | 0.0607 | Yes |
| 3.001 | 0.001022225 | 383.14 | 0.9393 | 0.0607 | Yes |
| 4.001 | 0.000744683 | 383.14 | 0.9393 | 0.0607 | Yes |
| 5.002 | 0.000581265 | 383.14 | 0.9393 | 0.0607 | Yes |
| 6.001 | 0.000472758 | 383.14 | 0.9393 | 0.0607 | Yes |
| 7.000 | 0.00039631 | 383.14 | 0.9393 | 0.0607 | Yes |
| 8.001 | 0.000339193 | 383.14 | 0.9393 | 0.0607 | Yes |
| 9.000 | 0.000294669 | 383.14 | 0.9393 | 0.0607 | Yes |
| 10.000 | 0.000259121 | 383.14 | 0.9393 | 0.0607 | Yes |
| 11.000 | 0.000230341 | 383.14 | 0.9393 | 0.0607 | Yes |
| 12.002 | 0.000206523 | 383.14 | 0.9393 | 0.0607 | Yes |
| 13.002 | 0.000186693 | 383.14 | 0.9393 | 0.0607 | Yes |
| 14.002 | 0.000169956 | 383.14 | 0.9393 | 0.0607 | Yes |
| 15.001 | 0.000155597 | 383.14 | 0.9393 | 0.0607 | Yes |
| 16.000 | 0.000143448 | 383.14 | 0.9393 | 0.0607 | Yes |
| 1.001 | 0.002503509 | 303.22 | 0.8709 | 0.1291 | Yes |
| 2.001 | 0.001180414 | 303.22 | 0.8709 | 0.1291 | Yes |
| 3.000 | 0.000746082 | 303.22 | 0.8709 | 0.1291 | Yes |
| 4.001 | 0.000530545 | 303.22 | 0.8709 | 0.1291 | Yes |
| 5.002 | 0.000398756 | 303.22 | 0.8709 | 0.1291 | Yes |
| 6.001 | 0.000309359 | 303.22 | 0.8709 | 0.1291 | Yes |
| 7.001 | 0.000242529 | 303.22 | 0.8709 | 0.1291 | Yes |
| 8.002 | 0.000190666 | 303.22 | 0.8709 | 0.1291 | Yes |
| 9.003 | 0.000148408 | 303.22 | 0.8709 | 0.1291 | Yes |
| 10.000 | 0.000114954 | 303.22 | 0.8709 | 0.1291 | Yes |
| 11.003 | 9.35623E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 12.003 | 8.09863E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 13.002 | 7.35001E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 14.004 | 6.86525E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 15.001 | 6.51449E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 16.003 | 6.26099E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 17.003 | 6.06296E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 18.005 | 5.89879E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 19.001 | 5.76081E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 20.001 | 5.64756E-05 | 303.22 | 0.8709 | 0.1291 | Yes |
| 1.004 | 0.002709605 | 323.18 | 0.8709 | 0.1291 | Yes |
| 2.002 | 0.001277746 | 323.18 | 0.8709 | 0.1291 | Yes |
| 3.004 | 0.000818891 | 323.18 | 0.8709 | 0.1291 | Yes |
| 4.006 | 0.000590453 | 323.18 | 0.8709 | 0.1291 | Yes |
| 5.001 | 0.000454064 | 323.18 | 0.8709 | 0.1291 | Yes |
| 6.001 | 0.000360989 | 323.18 | 0.8709 | 0.1291 | Yes |
| 7.002 | 0.000294265 | 323.18 | 0.8709 | 0.1291 | Yes |
| 8.002 | 0.000243712 | 323.18 | 0.8709 | 0.1291 | Yes |
| 9.002 | 0.000203887 | 323.18 | 0.8709 | 0.1291 | Yes |
| 10.001 | 0.000172089 | 323.18 | 0.8709 | 0.1291 | Yes |
| 11.000 | 0.000146463 | 323.18 | 0.8709 | 0.1291 | Yes |
| 12.001 | 0.000126071 | 323.18 | 0.8709 | 0.1291 | Yes |
| 13.000 | 0.000110259 | 323.18 | 0.8709 | 0.1291 | Yes |
| 14.001 | 9.82086E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 15.001 | 8.92738E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 16.002 | 8.25996E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 17.001 | 7.75544E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 18.001 | 7.35497E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 19.003 | 7.04477E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 20.001 | 6.78809E-05 | 323.18 | 0.8709 | 0.1291 | Yes |
| 1.000 | 0.002975439 | 343.15 | 0.8709 | 0.1291 | Yes |
| 2.003 | 0.001386207 | 343.15 | 0.8709 | 0.1291 | Yes |
| 3.001 | 0.000890136 | 343.15 | 0.8709 | 0.1291 | Yes |
| 4.001 | 0.000653424 | 343.15 | 0.8709 | 0.1291 | Yes |
| 5.001 | 0.000504569 | 343.15 | 0.8709 | 0.1291 | Yes |
| 6.006 | 0.000405032 | 343.15 | 0.8709 | 0.1291 | Yes |
| 7.003 | 0.00033541 | 343.15 | 0.8709 | 0.1291 | Yes |
| 8.005 | 0.00028312 | 343.15 | 0.8709 | 0.1291 | Yes |
| 9.000 | 0.000242778 | 343.15 | 0.8709 | 0.1291 | Yes |
| 10.001 | 0.000210446 | 343.15 | 0.8709 | 0.1291 | Yes |
| 11.001 | 0.000184158 | 343.15 | 0.8709 | 0.1291 | Yes |
| 12.002 | 0.000162636 | 343.15 | 0.8709 | 0.1291 | Yes |
| 13.002 | 0.000144814 | 343.15 | 0.8709 | 0.1291 | Yes |
| 14.003 | 0.00013012 | 343.15 | 0.8709 | 0.1291 | Yes |
| 15.001 | 0.000118028 | 343.15 | 0.8709 | 0.1291 | Yes |
| 16.003 | 0.000108119 | 343.15 | 0.8709 | 0.1291 | Yes |
| 17.001 | 0.000100065 | 343.15 | 0.8709 | 0.1291 | Yes |
| 18.001 | 9.35314E-05 | 343.15 | 0.8709 | 0.1291 | Yes |
| 19.001 | 8.81762E-05 | 343.15 | 0.8709 | 0.1291 | Yes |
| 20.001 | 8.37317E-05 | 343.15 | 0.8709 | 0.1291 | Yes |

Continued: Data summarised from Table 6 and 7 of Mantovani12 [109]

| P (MPa) | v ($\text{m}^3 \text{mol}^{-1}$) | T (K) | x_{CO_2} | x_{O_2} | Usable Data Point? |
|-----------|--------------------------------------|---------|-------------------|------------------|--------------------|
| 1.000 | 0.003185259 | 363.15 | 0.8709 | 0.1291 | Yes |
| 2.002 | 0.001473777 | 363.15 | 0.8709 | 0.1291 | Yes |
| 3.002 | 0.00095608 | 363.15 | 0.8709 | 0.1291 | Yes |
| 4.000 | 0.000701231 | 363.15 | 0.8709 | 0.1291 | Yes |
| 5.002 | 0.000547794 | 363.15 | 0.8709 | 0.1291 | Yes |
| 6.003 | 0.000444788 | 363.15 | 0.8709 | 0.1291 | Yes |
| 7.002 | 0.0003718 | 363.15 | 0.8709 | 0.1291 | Yes |
| 8.003 | 0.000317692 | 363.15 | 0.8709 | 0.1291 | Yes |
| 9.000 | 0.00027555 | 363.15 | 0.8709 | 0.1291 | Yes |
| 10.003 | 0.000241714 | 363.15 | 0.8709 | 0.1291 | Yes |
| 11.000 | 0.000214464 | 363.15 | 0.8709 | 0.1291 | Yes |
| 12.000 | 0.000191907 | 363.15 | 0.8709 | 0.1291 | Yes |
| 13.000 | 0.000173149 | 363.15 | 0.8709 | 0.1291 | Yes |
| 14.000 | 0.000157257 | 363.15 | 0.8709 | 0.1291 | Yes |
| 15.002 | 0.000143833 | 363.15 | 0.8709 | 0.1291 | Yes |
| 16.001 | 0.000132475 | 363.15 | 0.8709 | 0.1291 | Yes |
| 17.001 | 0.000122904 | 363.15 | 0.8709 | 0.1291 | Yes |
| 18.000 | 0.000114765 | 363.15 | 0.8709 | 0.1291 | Yes |
| 19.001 | 0.000107724 | 363.15 | 0.8709 | 0.1291 | Yes |
| 20.003 | 0.000101639 | 363.15 | 0.8709 | 0.1291 | Yes |
| 1.002 | 0.003586107 | 383.14 | 0.8709 | 0.1291 | Yes |
| 2.003 | 0.001638731 | 383.14 | 0.8709 | 0.1291 | Yes |
| 3.003 | 0.001046574 | 383.14 | 0.8709 | 0.1291 | Yes |
| 4.004 | 0.0007627 | 383.14 | 0.8709 | 0.1291 | Yes |
| 5.005 | 0.000596174 | 383.14 | 0.8709 | 0.1291 | Yes |
| 6.001 | 0.000486754 | 383.14 | 0.8709 | 0.1291 | Yes |
| 7.003 | 0.000408933 | 383.14 | 0.8709 | 0.1291 | Yes |
| 8.003 | 0.000351021 | 383.14 | 0.8709 | 0.1291 | Yes |
| 9.000 | 0.000306213 | 383.14 | 0.8709 | 0.1291 | Yes |
| 10.002 | 0.000270271 | 383.14 | 0.8709 | 0.1291 | Yes |
| 11.000 | 0.000241179 | 383.14 | 0.8709 | 0.1291 | Yes |
| 12.001 | 0.000217173 | 383.14 | 0.8709 | 0.1291 | Yes |
| 13.000 | 0.000197165 | 383.14 | 0.8709 | 0.1291 | Yes |
| 14.003 | 0.000180226 | 383.14 | 0.8709 | 0.1291 | Yes |
| 15.001 | 0.000165734 | 383.14 | 0.8709 | 0.1291 | Yes |
| 16.002 | 0.000153322 | 383.14 | 0.8709 | 0.1291 | Yes |
| 17.001 | 0.000142635 | 383.14 | 0.8709 | 0.1291 | Yes |
| 18.000 | 0.000133215 | 383.14 | 0.8709 | 0.1291 | Yes |
| 19.001 | 0.000125113 | 383.14 | 0.8709 | 0.1291 | Yes |
| 20.001 | 0.000118137 | 383.14 | 0.8709 | 0.1291 | Yes |

Continued: Data summarised from Table 6 and 7 of Mantovani12 [109]

7.2 Published Paper

Presented over the following eight pages our paper [40] published in May 2013 as part of the work done for this EngD. Its contents are broadly aligned with those which are presented in Chapter 4.

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